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COMPUTER SIMULATION OF THE CONTINUOUS
TNT PROCESS. VOLUME 1: THE NITRATION
SECTION

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SUMMARY

The development of a mathematical model of the nitration section of a continuous process for the manufacture of TNT is described. Implementation of the model on a high-speed digital computer is also discussed, as are the steady state and dynamic studies that were conducted on the resulting computer simulation. The way in which optimized process operating conditions and improved process control strategies were developed using the simulation is illustrated.

INTRODUCTION

Computer simulation of a chemical process, simply defined, is a procedure by which a mathematical model of the process' relevant chemical and physical characteristics is first constructed, after which the resultant system of equations is programmed for solution on a high speed computer. Such a model is usually based upon a combination of prevailing theory and empirical relationships, and, when properly formulated, will predict all process input/output relationships. The applicability of such a model depends heavily upon the ratio of theory to empiricism employed in model development. For example, a totally empirical model such as a least squares polynomial approximation is useful only within the boundaries of experimental observation, whereas a totally theoretical model, for example Newton's Laws of Motion as a description of projectile trajectories, will apply under virtually all conditions. For most complex systems (such as a chemical process) an optimum balance between theory and observation must be sought.

Upon completion of mathematical modeling and computer programming, the resulting computer simulation can then, after verification against real process data, be used to study the process without incurring the cost, time loss, and (especially in the case of explosives manufacturing processes) the risk involved in pilot plant or full-scale plant experimentation. Most often, studies of both the static and dynamic states of the process are carried out, the objective of the former being optimization of operating and design conditions, and the objective of the latter being development and testing of control strategies.

It has always been possible to develop mathematical models of complex physical systems. However, the value of such models remained questionable until the application of digital, analog, and hybrid computers made possible the rapid solution of the complex equations which usually resulted. It has only been in the last 10 to 15 years that mathematical modeling of complex processes has yielded significant accomplishments. Most notable among these have been the simulations used in the aerospace industry, especially in the manned space flight program.

Although employed successfully as a process study tool for a number of years in private industry, the application of chemical process simulation to the U. S. Army Armament Command's explosive and propellant manufacturing processes is just now beginning to be appreciated. For the past three and a half years, the Chemical Process Technology Division of the

Manufacturing Technology Directorate at Picatinny Arsenal has been engaged in an extensive effort to improve, via the application of computer simulation, a continuous process for TNT manufacturing. This work has been carried out jointly with Imperial Chemical Industries, U. S. (ICIUS) the operating contractor at Volunteer Army Munition Plant in Chattanooga, Tennessee, and has to date gone through three distinct phases: Phase I, initial development of a kinetics and mass transfer model of the nitration section with subsequent implementation on a hybrid computer; Phase II, conversion of the hybrid nitration model to a pure digital model, followed by improvement of the nitration model based on new plant data and additional theoretical considerations, simulation of nitration section hydraulics, and development of a simulation of the purification section of the process; and Phase III, extensive exploitation of the nitration and purification computer models.

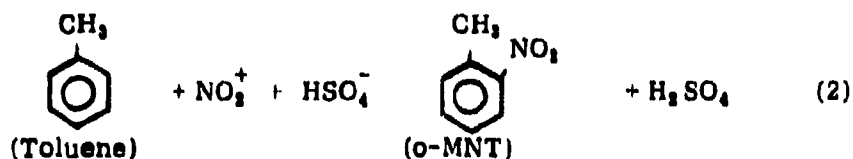
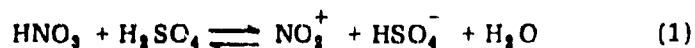
Project summary reports (Ref 1, 2, 3) have previously been prepared covering these efforts. However, no unified text has been generated which ties together all the interrelated tasks and provides a much needed explanation of the present structure, capabilities, and limitations of various models developed. The purpose of this report is to satisfy these needs as well as to clarify material in the existing reports which has either become outdated or which the author feels is unclear as presently stated.

Because of the extensive amount of information which is presented, the report has been prepared in three volumes. Volume I describes the modeling and simulation effort that has been carried out on the nitration section of the process, including a description of the process chemistry and equipment. Volume II deals exclusively with the purification section model, and Volume III involves the simulation of the hydraulic phenomena occurring in a nitration stage.

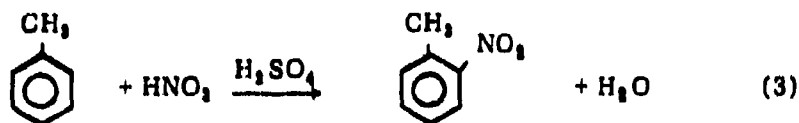
THE CHEMISTRY OF TNT NITRATION - A BRIEF DESCRIPTION

The production of TNT is essentially carried out via a three-step reaction in which toluene and its mono- and dinitro-substituted derivatives are contacted with mixtures of nitric and sulfuric acid called mixed acid. Each step in the reaction corresponds to the successive electrophilic substitution of a hydrogen ion (H^+) by a nitronium ion (NO_2^+) on the aromatic ring of the toluene molecule. The nitric acid serves as the source of NO_2^+ ions, while the sulfuric acid acts as both a catalyst and dehydrating agent, first reacting with the nitric acid to generate NO_2^+ ions and then picking up the water which forms as a product of the nitration reaction.

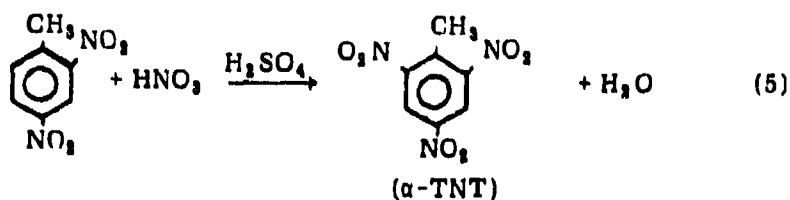
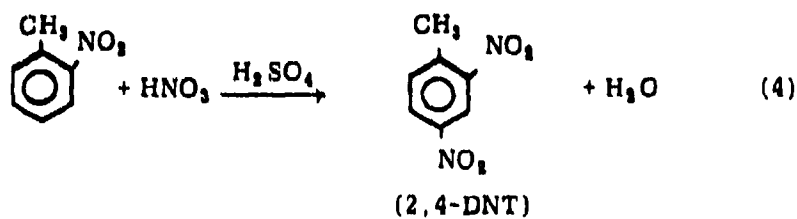
A simplified scheme for the mononitration of toluene in mixed acid can be written as follows:



Adding reactions 1 and 2 gives the overall reaction:

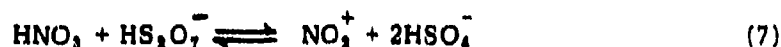
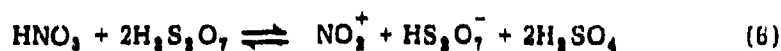


Similarly, when toluene is replaced by mononitrotoluene (MNT) or dinitrotoluene (DNT), the stoichiometric reactions are written as



The temperature as well as the composition of mixed acid required to efficiently carry out each of the above reactions is different, reflecting the relative ease with which nitration is accomplished. Thus, Reaction 3 is usually conducted at relatively low temperatures (40° to 50°C) with weak acid solutions, while reactions 4 and 5 require progressively higher temperatures (60° to 100°C) and stronger acid mixtures to be driven to the desired degree of completion.

The strength of mixed acid is usually determined by the amount of water present. In aqueous media Reaction 1 controls the generation of nitronium ions. However, when nitration is conducted in an anhydrous medium, the acid mixture consists of nitric acid and oleum (100% H₂SO₄ in which SO₃ dissolved) and the controlling nitronium ion generation equilibria are:



It is also worth noting that Reactions 3, 4, and 5 are highly exothermic.

Although not shown in Reactions 3 through 5, a significant amount of isomerism occurs, resulting in the production of a variety of nitrated components in addition to the desired α -TNT. A complete description of the isomerism in toluene nitration with relative amounts of each component formed is given in Figure 1. The relative amounts of isomers formed depend upon nitrating temperature and acid composition. Thus Figure 1 must be viewed as a typical distribution only. In the continuous TNT process at Radford Army Ammunition Plant, only the α , β , γ , and ϵ isomers have been positively identified, although by the analytical technique used on process samples, it is not possible to separate the α and η isomers (Ref 4).

In addition to its function as a nitrating agent, nitric acid also plays the role of an oxidant under the usual conditions found in toluene nitration reactions. All nitrated components are capable of undergoing some form of oxidation. Two types of oxidation reactions are observed: those which result in destruction of the aromatic ring, yielding gaseous products, and those which result in oxidation of the methyl group or hydroxylation of the aromatic ring, yielding stable organic compounds. Typically, MNT undergoes hydroxylation to the cresol which is later destructively oxidized to gaseous products; DNT undergoes complete ring destruction

to yield CO_2 , CO , NO , NO_2 and tetranitromethane (TNM); and TNT undergoes methyl group oxidation to yield a variety of organic products as shown in Figure 2.

In a typical nitration of toluene to TNT, isomerism and oxidation account for a yield loss of about 8 to 10% based on molar feed of toluene.

PROCESS DESCRIPTION

The continuous TNT process, which is the subject of the simulation study, is an adaptation of technology developed by Canadian Industries Limited and is currently the only continuous process for manufacture of TNT operating in the United States.

Nitration is carried out in a series of six reaction stages, each consisting of a 425-gallon nitrator and a 150-gallon separator, except for Stages 1 and 3 which have two nitrators. Because of the ratios of mixed acid to toluene employed in the process, a two-phase system results, with nitration occurring in the acid phase as diffusion and solubility phenomena establish equilibrium concentrations of the organic species in that phase. Separation of organic and acid phases is carried out after each nitration stage and enables countercurrent flow of the reactants to be maintained. A flow diagram of the nitration section of the process is shown in Figure 3, and a detailed diagram of a nitrator/separator nitration stage is shown in Figure 4.

In the countercurrent process, all of the toluene is introduced into the first stage, where mononitration and a small amount of dinitration occurs. After separation, this so-called "nitrobody" stream moves forward through the reactor train, becoming more highly nitrated as it progresses from vessel to vessel. Oleum is fed to Stage 6 and by means of the mixed acid recycle streams, moves in the opposite direction, decreasing in strength as it flows toward Stage 1. Nitric acid is added to each stage in order to maintain the correct mixed acid composition. Mixed acid recycle streams also contain some dissolved nitrobody as well as nitrosylsulfuric acid (HNO_2SO_4) which forms as a result of the oxidation side reactions.

As pointed out previously, nitration becomes progressively more difficult as the number of nitro groups on the aromatic ring of the substrate increases. Thus, the temperature as well as the mixed acid strength

must increase from Stage 1 to Stage 6. Nominal temperatures for the eight nitrators are 55, 50, 70, 80, 85, 90, 95, and 100°C respectively.

From Figure 4 it is seen that a nitrator is a cylindrically shaped vessel with an agitator fitted inside a draft tube at the center. The agitator provides the required interphase mixing in the nitrator and also creates a head difference between material on either side of the draft tube which in turn provides the motive force for fluid flow. There are no pumps in the system. Rapid internal circulation of material over the nitrator's cooling coils is maintained. There is also a recycle of acid between the separator and its own nitrator (internal recycle). Flow of this stream can be adjusted to maintain proper cooling in the separator or to change the acid-to-nitrobody ratio and residence time in the nitrator.

The acid stream flowing from a separator to the previous nitration stage (external recycle) passes through a weir-like device called a decanter. By adjusting this apparatus, the nitrobody/acid interface in the separator can be regulated to insure adequate phase separation. However, under normal operating conditions of 55 tons per day TNT production, a significant amount of entrainment still occurs, especially in Separator 3.

The crude TNT leaving Separator C flows to the purification section where residual nitrating acid and asymmetrical isomers are removed prior to final packaging of the product.

DEVELOPMENT OF THE MATHEMATICAL MODEL

The Single Vessel Model

The majority of the work conducted under the TNT process computer simulation effort has been devoted to the construction of a mathematical model which describes the nitration section of the process in terms of the kinetic and mass transfer phenomena which are believed to occur there and account for most of the process' behavior. As previously indicated, models of the purification section and of the hydraulic phenomena which govern fluid flow in a given nitration stage have also been developed but will not be discussed in this volume.

The kinetic and mass transfer model of the nitration section of the process (hereafter called the nitration section model) is the end product of numerous refinements and improvements which have been made to a first-generation model developed for Picatinny Arsenal in May 1970 by Kinotrol, Inc. of Houston, Texas, functioning as a consultant to ICIUS at Volunteer Army Ammunition Plant in Chattanooga, Tennessee. The structure and contents of the original nitration section model can be found in Reference 1.

As in the original, a fundamental approach was taken in developing the present nitration section model. Wherever possible, theoretical equations are employed to represent the chemical and physical phenomena which govern the nitration process. The use of empirically derived equations and correlations is kept to a minimum and has been resorted to only after exhaustive research for theoretical alternatives proved fruitless. Phenomena described by the model include kinetics of nitration and oxidation of organic species, diffusion of the organic species between the acid and organic phases, solubility of organic species in the acid phase, and solubility of nitric acid in the organic phase. The way in which real plant data was used in the development of the nitration section model will be described when parameter fitting is explained in a later section of this report.

The easiest way to explain the nitration section model is to take a single vessel in the nitration train (there are 14 vessels in series) and develop a complete material balance for each component in both acid and organic phases. The generalized nitrator in Figure 5 showing actual stream flows could be used for this purpose. However, the analysis is far simpler if each stream is broken down into its acid and organic phases with the subsequent addition of similar phases, so that the vessel input and output consist of a single acid phase, A, a single organic phase P, and a gas phase, G. Figure 6 illustrates this simplifying concept. Thus, for component i in the acid phase, a mole balance can be written as:

$$\begin{aligned}
 &(\text{Rate of moles } i \text{ in with } A_0) + \\
 &(\text{Rate of generation of moles } i \\
 &\quad \text{in the acid phase within} \\
 &\quad \text{nitrator } n) - \\
 &(\text{Rate of moles } i \text{ out with } A_n)
 \end{aligned}
 =
 \begin{aligned}
 &(\text{Rate of accumulation of} \\
 &\text{moles } i \text{ within the acid} \\
 &\text{of nitrator } n)
 \end{aligned}
 \quad (1)$$

The balance for component i in the organic phase follows the same form as Equation 1. For the gas phase, the balance is simplified by the fact that products of the gaseous reaction are insoluble in both the acid and organic phases. Thus,

$$\begin{array}{l} \text{(Rate of generation of} \\ \text{gaseous species } i \text{ in} \\ \text{nitratator } n) \end{array} = \begin{array}{l} \text{(Rate of gaseous } i \text{ out} \\ \text{with } G_n) \end{array} \quad (2)$$

For a specific component, say α -TNT, the molar balances for vessel n are written as:

$$A_{n,\alpha\text{-TNT}}^O + \Sigma S_{n,\alpha\text{-TNT}}^A - A_{n,\alpha\text{-TNT}} = \frac{dA_{n,\alpha\text{-TNT}}}{dt} \quad (3)$$

for the acid phase, where S^A is the acid phase generation term, and

$$P_{n,\alpha\text{-TNT}}^O + \Sigma S_{n,\alpha\text{-TNT}}^P - P_{n,\alpha\text{-TNT}} = \frac{dP_{n,\alpha\text{-TNT}}}{dt} \quad (4)$$

for the organic phase, where S^P is an organic phase generation term. The assumption of a perfectly backmixed reactor allows for the equivalency of the reactor contents and the reactor outflow.

Equations similar to 3 and 4 can be written for all the components in each phase for every vessel in the nitration train. In the current version of the nitration section model, 10 chemical components are considered in the organic phase, 14 in the acid phase, and 3 in the gaseous effluent (see Figure 8). Before proceeding further, a few comments on these components are in order. First, all nitrobody components originating from m -MNT have been lumped together in the m -DNT and m -TNT terms in order to simplify the kinetics of the asymmetrical isomer reactions. Secondly, a single term, TNBX, is used to represent all components other than TNB formed from methyl group oxidation of TNT. This includes trinitrobenzyl alcohol, trinitrobenzaldehyde, and trinitrobenzoic acid. Lumping of oxidation products into one term was necessitated by a lack of process data for these components, and is justified considering the small concentration of each component which is present.

Thus, from Equations 3 and 4, it can be seen that for a given vessel the model consists essentially of a series of first order, non-linear, coupled, ordinary differential equations which make up the vessel's material balance.

The way in which the individual vessels are connected and the procedure for generating the flow and composition of the actual process streams from the ideal phases will be discussed at length in later sections of this report.

The heart of the vessel material balance equations and therefore the heart of the nitration section model is the generation terms. These terms are actually equations which represent the kinetic, mass transfer, and solubility processes occurring within a given vessel. For each component balance equation, three generation terms exist: reaction rate ($R_{n,i}$), diffusion ($D_{n,i}$), and bulk mass transport ($M_{n,i}$).

Thus Equation 3 can be rewritten as:

$$A_{n,\alpha\text{TNT}}^O + R_{n,\alpha\text{TNT}}^A + D_{n,\alpha\text{TNT}}^A + M_{n,\alpha\text{TNT}}^A - A_{n,\alpha\text{TNT}} = \frac{dA_{n,\alpha\text{TNT}}}{dt} \quad (5)$$

Since it is widely accepted that all reactions occur in the acid phase, it follows that $R_{n,i}^P = 0$. Also mass transfer into the acid phase must be at the expense of material in the organic phase so that $D_{n,\alpha\text{TNT}}^P = -D_{n,\alpha\text{TNT}}^A$ and $M_{n,\alpha\text{TNT}}^P = -M_{n,\alpha\text{TNT}}^A$. Thus, Equation 4 can be written as:

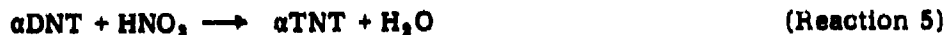
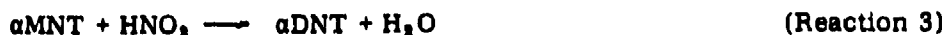
$$P_{n,\alpha\text{TNT}}^O - D_{n,\alpha\text{TNT}} - M_{n,\alpha\text{TNT}} - P_{n,\alpha\text{TNT}} = \frac{dP_{n,\alpha\text{TNT}}}{dt} \quad (6)$$

Note that there is no longer a need for acid and organic phase superscripts on the mass transfer terms. Development of the generation terms $R_{n,i}^A$, $D_{n,i}$, and $M_{n,i}$ will now be discussed in detail.

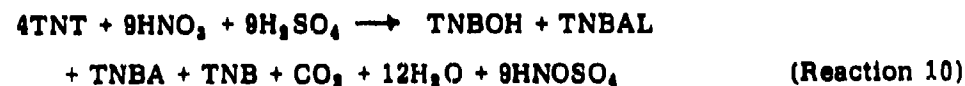
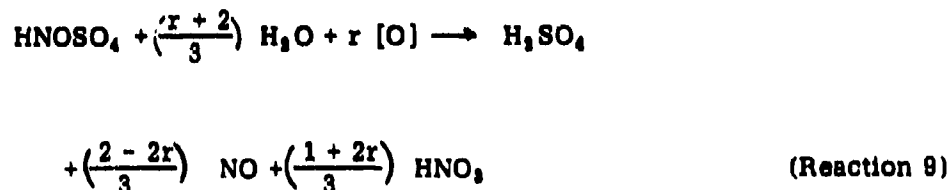
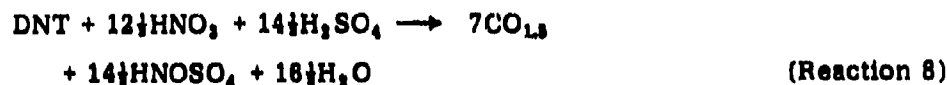
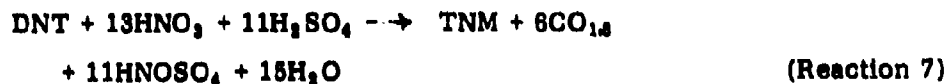
Reaction Kinetics

Reaction rate expressions have been developed to represent the nitration and oxidation of toluene and its nitro-substituted derivatives at each stage in the reactor train. The stoichiometric reactions which are considered in the nitration section model include:

Nitration



Oxidation



It is pointed out that Reactions 1 through 10 are not mechanistic equations but rather stoichiometric equations which account for the appearance and disappearance of the various chemical components during the nitration process.

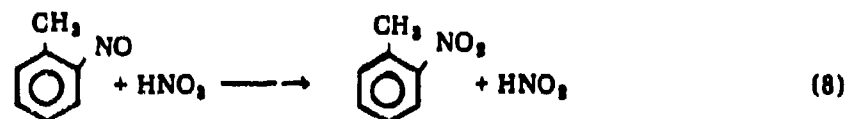
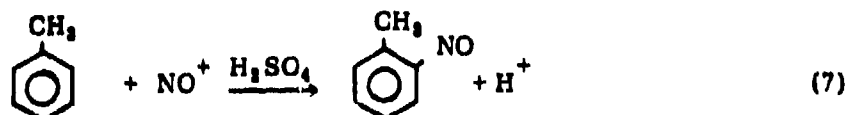
As mentioned briefly in the section on process chemistry, aromatic nitration in mixed acid occurs via electrophilic substitution, where in most instances the electrophile has been proven to be the nitronium ion.

However, it has also been well established (Ref 6) that as the molar ration of water to sulfuric acid in the mixed acid increases to unity, the

concentration of NO_2^+ falls off rapidly to nearly spectroscopically undetectable levels. Thus, in the case where $[\text{H}_2\text{O}]/[\text{H}_2\text{SO}_4] > 1$ (the weak acid region) and nitration is still seen to occur at a rapid rate, either the aromatic substrate is reactive enough to require only trace amounts of nitronium ion for reaction to proceed, or another nitration mechanism, say one dependent on molecular nitric acid is in effect. The former is more likely but the latter cannot be ruled out.

In the continuous TNT process, all of the monitration and a significant amount of dinitration occurs in mixed acid where $[\text{H}_2\text{O}]/[\text{H}_2\text{SO}_4] > 1$, so that in developing a kinetics model for this weak acid region one of the two mechanism hypothesis must be chosen. It was first decided to test both hypotheses against actual process performance data. While the nitronium ion mechanism was eventually shown to be preferable and was subsequently included in the overall nitration section model, a detailed description at the weak acid model based on molecular nitric acid is nevertheless also presented here for reasons of completeness.

The molecular nitric dependent weak acid kinetics model was based on the work of Kobe and Lakemeyer (Ref 7) and McKinley and White (Ref 8) who investigated the factors affecting the mononitration of toluene in mixed acid where the molar ratio of water to sulfuric acid was greater than two. A mechanism is proposed whereby the nitrosonium ion, NO^+ , is first formed, then attacks the benzene ring and is subsequently oxidized by nitric acid to yield the mononitrated product. This mechanism can be represented as follows:



Although not definitively stated in the literature, Equation 8 appears to be the rate limiting step since data taken by McKinley and White show a strong dependence on the concentration of molecular nitric acid in the acid phase. McKinley and White's nitration studies also indicate that the sulfuric acid concentration has a significant influence on the rate of toluene

nitration in weak acid. Finally, Kobe and Lakemeyer demonstrated that the presence of nitrosylsulfuric acid in weak nitrating acid mixtures causes a maximum in the rate at 4 mole % HNOSO_4 .

All of the above observed behavior was combined to yield an expression for the bimolecular rate constant for nitration in weak acid. This expression should be applicable to toluene, MNT, or DNT as long as the conditions of a weak acid nitrating medium are met. The form of this expression is:

$$\text{Rate}_N = \frac{d[N]}{dt} = k_2 [\text{HNO}_3] [M] \quad (9)$$

$$k_2 = [\text{H}_2\text{SO}_4]^c 10^{-a^2} (x_{\text{HNOSO}_4} - .04)^2 \quad (10)$$

where $[M]$ is the concentration of the organic reactant in the acid phase;
 $[N]$ is the concentration of the organic product in the acid phase;
 x_{HNOSO_4} is the mole fraction nitrosylsulfuric acid in the acid phase;
 and a and c are adjustable parameters.

The dependence of weak acid nitration reactions on temperature was expressed through an Arrhenius-type relationship and, reaction was limited to the acid phase. Thus, Equations 9 and 10 can be restated as:

$$\text{Rate}_N = \frac{d[N]}{dt} = k_N e^{-\frac{E_N}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)} [M] \delta \quad (11)$$

$$\delta = V_a [\text{HNO}_3] [\text{H}_2\text{SO}_4]^c 10^{-a^2} (x_{\text{HNOSO}_4} - .04)^2 \quad (12)$$

where V_a is the volume of the acid phase;
 k_N is the Arrhenius frequency factor;
 E_N is the activation energy; and
 T_R is a reference temperature.

Plant data for the continuous process at Radford indicates that toluene will react to mononitrotoluene just as fast as it can diffuse into the acid phase. Thus for Reactions 1 and 2, mass transfer is the limiting factor and the weak acid kinetics developed above are of academic interest only. However, for conversion of MNT to DNT in weak acid, the weak acid mechanism would apply.

The above model is obviously based on rather unstable theoretical grounds and even though a reasonably good fit to plant data was achieved with it, it was scrapped in favor of a more theoretically consistent nitronium ion dependent system of equations.

In this approach the reaction rate is still expressed as in Equation 9; however the expression for k_2 is simply:

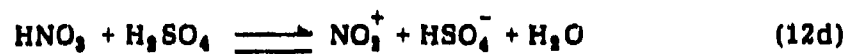
$$k_2 = V_a K_N Q \quad (12a)$$

where:

$$K_N = k_N e^{-\frac{E_N}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)} \quad (12b)$$

$$Q = \frac{[NO_2^+]}{[HNO_3]} \quad (12c)$$

Utilization of this model depends on the ability to compute the nitronium concentration from the equilibrium reactions which are in effect. The controlling equilibria are chosen to be (Ref 18):



The procedure by which the NO_3^+ concentration is calculated follows below.

In the weak acid region, the initial and equilibrium concentrations are given as:

<u>Component</u>	<u>Initial</u>	<u>At Equilibrium</u>
HNO_3	$[\text{HNO}_3]_0$	$[\text{HNO}_3]$
H_2SO_4	$[\text{H}_2\text{SO}_4]_0$	$[\text{H}_2\text{SO}_4]$
H_2O	$[\text{H}_2\text{O}]_0$	$[\text{H}_2\text{O}]$
NO_3^+	0	$[\text{NO}_3^+]$
H_3O^+	0	$[\text{H}_3\text{O}^+]$
HSO_4^-	0	$[\text{HSO}_4^-]$

By writing material balances for each chemical element, a system of equations can be developed which, in conjunction with the equilibrium Equations 12d and 12e, can be used to solve for the desired NO_3^+ concentration at equilibrium. The elemental material balances are based on the necessary equivalence of the moles of chemical elements present initially and the moles of chemical elements present at equilibrium.

For Nitrogen:

$$[\text{HNO}_3]_0 = [\text{HNO}_3] + [\text{NO}_3^+] \quad (12f)$$

For Sulfur:

$$[\text{H}_2\text{SO}_4]_0 = [\text{H}_2\text{SO}_4] + [\text{HSO}_4^-] \quad (12g)$$

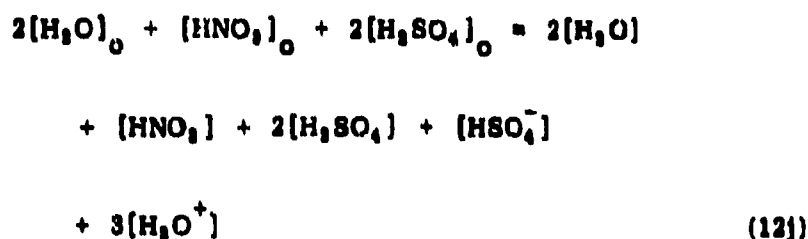
For Oxygen:

$$\begin{aligned} [\text{H}_2\text{O}]_0 + 3[\text{HNO}_3]_0 + 4[\text{H}_2\text{SO}_4]_0 &= [\text{H}_2\text{O}] \\ &+ 3[\text{H}_2\text{O}] + 4[\text{H}_2\text{SO}_4] + 2[\text{NO}_3^+] \\ &+ 4[\text{HSO}_4^-] + [\text{H}_3\text{O}^+] \end{aligned} \quad (12h)$$

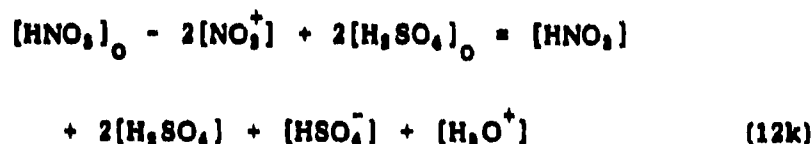
Making use of Equations 12f and 12g in Equation 12h gives:



For Hydrogen:



Multiplying Equation 12i by 2 and subtracting from Equation 12j gives:



And subtracting Equations 12f and g from Equation 12k and gives:



Now, let the initial concentrations be given as:

$$[\text{H}_2\text{O}]_0 = W$$

$$[\text{H}_2\text{SO}_4]_0 = S$$

$$[\text{HNO}_3]_0 = F$$

and the equilibrium concentrations of nitronium and bisulfate ions be given as x and y respectively. Then at equilibrium, the concentration of the remaining components can be expressed as:

$$[\text{HNO}_3] = F - x \quad (\text{from Eq 12f})$$

$$[\text{H}_2\text{SO}_4] = S - y \quad (\text{from Eq 12g})$$

$$[\text{H}_3\text{O}^+] = y - x \quad (\text{from Eq 12h})$$

$$[\text{H}_2\text{O}] = W + x - (y - x) \quad (\text{from Eq 12i})$$

The equilibrium constant for Equation 12d is given by:

$$K_1 = \frac{[\text{NO}_3^+][\text{HSO}_4^-][\text{H}_2\text{O}]}{[\text{H}_2\text{SO}_4][\text{HNO}_3]} = \frac{(x)(y)(W+2x-y)}{(S-y)(F-x)} \quad (13)$$

and that for Equation 12e by:

$$K_2 = \frac{[\text{H}_3\text{O}^+][\text{HSO}_4^-]}{[\text{H}_2\text{O}][\text{H}_2\text{SO}_4]} = \frac{(y-x)(y)}{(W+2x-y)(S-y)} \quad (14)$$

Based on the impossibility of negative concentrations, the assumed existence of all possible components at equilibrium, the following constraints must apply:

$$\begin{array}{ll} 0 < x < y & \text{if } y < F \\ 0 < x < F & \text{if } F < y \\ 0 < y < (W+2x) & \text{if } (W+2x) < S \\ 0 < y < S & \text{if } S < (W+2x) \end{array}$$

Knowing K_1 , K_2 , F , W , and S , and utilizing the above constraints, Equations 13 and 14 can be solved for x , the nitronium ion concentration at equilibrium. From Equation 14,

$$x = \frac{y^2 - K_2(S-y)(W-y)}{2K_2(S-y) + y} \quad (15)$$

Equation 15 can be solved for x and y by an interval halving procedure after which the solution values can be substituted in Equation 13 to give

a value of K_1 . If convergence on K_1 is not achieved, the procedure is repeated using the current value of y to adjust the upper or lower boundary of the solution interval for x . In actual execution of the model, between 20 and 40 iterations are required to converge on K_1 for each pass through the vessel equations.

Before moving on to the strong acid region it should be pointed out that a general mechanism for aromatic nitration in aqueous mixed acid has been proposed (Ref 9) based on activity coefficients, but lack of data prevented using it in the nitration section model. An attempt was made, however, to do without any theoretically based weak acid mechanism and just use a curve fit of laboratory data developed by Vinnik (Ref 10) for nitration of p-MNT in mixed acid. The lower end of the curve had to be extrapolated since no data was provided for H_2SO_4 concentrations less than 80%. In all cases, the weak acid mechanism of Equations 9, 12a, 12b and 12c gave far better agreement with observed plant behavior, and it is these equations that constitute the current model.

For strong acid nitration (i.e. $[H_2O]/[H_2SO_4] < 1$) it is firmly established that the nitronium ion is the active nitrating species. Bennett (Ref 11) developed an expression for the bimolecular nitration rate constant, k_2 , in the reaction

$$\frac{d[TNT]}{dt} = k_2 [HNO_2^+][DNT] \quad (16)$$

where the dependence on the NO_2^+ ion concentration as well as the concentration of proton acceptor components (HSO_4^- , H_2SO_4 , and $HS_2O_7^-$) are considered. Bennett's expression is given as follows:

$$k_2 = Q \left(k' [HSO_4^-] + k'' [H_2SO_4] + k''' [HS_2O_7^-] \right) \quad (17)$$

$$\text{where } Q = \frac{[NO_2^+]}{[HNO_2^+]}$$

In order to use Bennett's equation to represent strong acid nitration it is necessary to determine the nitronium and proton acceptor ion concentrations throughout the nitration section of the process. In the model, four strong acid regions are defined in which these ions should exist, and

then equilibrium equations are established which allow calculation of the ionic component concentrations. The first two regions are exactly those dealt with by Bennett. However the third and fourth regions have apparently never been examined experimentally so that the hypothesis presented below constitutes an extension of existing theory.

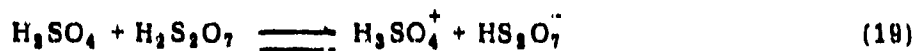
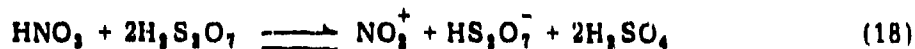
The first region (aqueous region) is characterized by the presence of water subject to the constraint $[H_2O]/[H_2SO_4] < 1$. The equilibria established in this situation are exactly those of Equations 12d and 12e for which the procedure to determine the equilibrium concentrations has been given.

The remaining three regions are water free, with nitric, sulfuric, and pyrosulfuric ($H_2S_2O_7$) acids making up the nitrating acid. These will be referred to as oleum regions.

In the first oleum region (nitric limited), pyrosulfuric acid is in large excess of the nitric acid to the extent that

$$[HNO_3] \leq .5 [H_2S_2O_7]$$

This is the strong oleum region described by Bennett. The equilibria governing concentrations in this region are:



Equation 18 is believed to go completely to the right, thus leaving Equation 19 as the limiting equilibrium. A two-step reaction occurs, the nitric acid first completely dissociating to nitronium ions via Equation 18, followed by the establishment of equilibrium among sulfuric, pyrosulfuric acids and their ionic counterparts via Equation 19. The concentrations are represented as follows:

	Initial	After 18	After 19 (Equilibrium)
HNO ₃	[HNO ₃] ₀	0	0
H ₂ S ₂ O ₇	[H ₂ S ₂ O ₇] ₀	[H ₂ S ₂ O ₇] ₀ - 2[HNO ₃] ₀	[H ₂ S ₂ O ₇] ₀ - 2[HNO ₃] ₀ - Y
H ₂ SO ₄	[H ₂ SO ₄] ₀	[H ₂ SO ₄] ₀ + 2[HNO ₃] ₀	[H ₂ SO ₄] ₀ + 2[HNO ₃] ₀ - Y
HS ₂ O ₇ ⁻	0	[HNO ₃] ₀	[HNO ₃] ₀ + Y
NO ₃ ⁺	0	[HNO ₃] ₀	[HNO ₃] ₀
H ₃ SO ₄ ⁺	0	0	Y

where Y is the concentration of HS₂O₇⁻ formed via Equation 19. The mass action expression for Equation 19 is:

$$K_{eq} = \frac{[H_2SO_4]^+ [HS_2O_7]^-}{[H_2SO_4] [H_2S_2O_7]} \quad (20)$$

Substitution of the tabulated values yields:

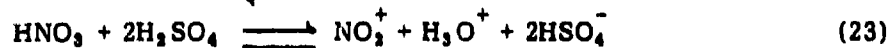
$$K_{eq} = \frac{Y ([HNO_3]_0 + Y)}{([H_2SO_4]_0 + 2[HNO_3]_0 - Y) ([H_2S_2O_7]_0 - 2[HNO_3]_0 - Y)} \quad (21)$$

If K_{eq} and initial concentrations are known, Y can be found by successive iterations of Equation 21. Bennett has suggested a value of 1.0 for K_{eq} .

In the second oleum region (intermediate), the pyrosulfuric acid is in moderate excess of the nitric such that:

$$.5[H_2S_2O_7] < [HNO_3] \leq [H_2S_2O_7]$$

The dominant equilibria in effect here are (Ref 19):



Again it is assumed that Equation 22 goes completely to the right. Because of the limits imposed on the nitric acid concentration, it must be true that the nitric acid remaining undissociated after reacting with $\text{H}_2\text{S}_2\text{O}_7$ (Eq 22) must always be less than the HS_2O_7^- formed by the same reaction. Thus, there will always be enough HS_2O_7^- present to soak up all of the H_2O^+ formed via equilibrium Equation 23. This continuously drives Equation 23 to the right until all the remaining nitric acid is completely converted to nitronium ions. Equations 23 and 24 can be added to give



In effect a two-step reaction occurs. Nitric acid reacts with the pyrosulfuric acid via Equation 22, and then the remaining undissociated nitric acid reacts completely with the HS_2O_7^- produced from the first reaction. Both reactions go to completion and no equilibria are in effect. Concentrations are as follows:

	Initial	After 22	After 25
$\text{H}_2\text{S}_2\text{O}_7$	$[\text{H}_2\text{S}_2\text{O}_7]_0$	0	0
H_2SO_4	$[\text{H}_2\text{SO}_4]_0$	$[\text{H}_2\text{SO}_4]_0 + [\text{H}_2\text{S}_2\text{O}_7]_0$	$[\text{H}_2\text{SO}_4]_0 + [\text{H}_2\text{S}_2\text{O}_7]_0$
NO_2^+	0	$.5[\text{H}_2\text{S}_2\text{O}_7]_0$	$[\text{HNO}_3]_0$
HS_2O_7^-	0	$.5[\text{H}_2\text{S}_2\text{O}_7]_0$	$[\text{H}_2\text{S}_2\text{O}_7]_0 - [\text{HNO}_3]_0$
HSO_4^-	0	0	$2[\text{HNO}_3]_0 - [\text{H}_2\text{S}_2\text{O}_7]_0$
HNO_3	$[\text{HNO}_3]_0$	$[\text{HNO}_3]_0 - .5[\text{H}_2\text{S}_2\text{O}_7]_0$	0

While Gillespie maintains that Equation 25 is completely to the right, there is some basis for the occurrence of the reverse reaction (Ref 20). For this reason, the model has been structured so that, as an option, Equation 25 can be treated as an equilibrium with

$$K_{\text{eq}} = \frac{[\text{HNO}_3][\text{HS}_2\text{O}_7^-]}{[\text{NO}_2^+][\text{HSO}_4^-]^2} \quad (25a)$$

Initial concentrations are assumed to be those existing after Equation 25 has gone completely to right at which time NO_2^+ and HSO_4^- begin to recombine via the reverse reaction. Equilibrium concentrations are found by assuming a value for K_{eq} and solving Equation 25a by interval halving.

In the third oleum region (oleum limited), nitric acid exists in excess of pyrosulfuric acid, i.e. $[\text{HNO}_3] > [\text{H}_2\text{S}_2\text{O}_7]$. The same equilibria are in effect here as in the intermediate region, but now Equation 25 can apply only until the HS_2O_7^- produced by Equation 22 is completely dissipated. There will still be some undissociated nitric remaining which must then undergo equilibrium dissociation via Equation 23. In effect, a three-step reaction takes place: 1) Nitric acid $\rightarrow \text{NO}_2^+$ in the presence of $\text{H}_2\text{S}_2\text{O}_7$, 2) Nitric acid $\rightarrow \text{NO}_2^+$ via Equation 25 until all the HS_2O_7^- is dissipated, and 3) Equilibrium dissociation of the remaining nitric acid via Equation 23. Concentrations are as follows:

	Initial	After 22	After 25	After 23 (Equilibrium)
HNO_3	$[\text{HNO}_3]_0$	$[\text{HNO}_3]_0 - .5[\text{H}_2\text{S}_2\text{O}_7]_0$	$[\text{HNO}_3]_0 - [\text{H}_2\text{S}_2\text{O}_7]_0$	$[\text{HNO}_3]_0 - [\text{H}_2\text{S}_2\text{O}_7]_0 - x$
$\text{H}_2\text{S}_2\text{O}_7$	$[\text{H}_2\text{S}_2\text{O}_7]_0$	0	0	0
H_2SO_4	$[\text{H}_2\text{SO}_4]_0$	$[\text{H}_2\text{SO}_4]_0 + [\text{H}_2\text{S}_2\text{O}_7]_0$	$[\text{H}_2\text{SO}_4]_0 + [\text{H}_2\text{S}_2\text{O}_7]_0$	$[\text{H}_2\text{SO}_4]_0 + [\text{H}_2\text{S}_2\text{O}_7]_0 - 2x$
NO_2^+	0	$.5[\text{H}_2\text{S}_2\text{O}_7]_0$	$[\text{H}_2\text{S}_2\text{O}_7]_0$	$[\text{H}_2\text{S}_2\text{O}_7]_0 + x$
HS_2O_7^-	0	$.5[\text{H}_2\text{S}_2\text{O}_7]_0$	0	0
HSO_4^-	0	0	$[\text{H}_2\text{S}_2\text{O}_7]_0$	$[\text{H}_2\text{S}_2\text{O}_7]_0 + 2x$
H_3O^+	0	0	0	x

where z is the concentration of nitronium ions formed via the equilibrium Equation 23.

As before, the mass action expression for Equation 23 is:

$$K_{eq} = \frac{[NO_2^+][H_2O^+][HSO_4^-]^2}{[HNO_3][H_2SO_4]^2} \quad (26)$$

Substitution of the appropriate tabulated values into Equation 26 gives:

$$K_{eq} = \frac{([H_2S_2O_7]_0 - z)(z)([H_2S_2O_7]_0 + 2z)^2}{([HNO_3]_0 - [H_2S_2O_7]_0 - z)([H_2SO_4]_0 + [H_2S_2O_7]_0 - 2z)^2} \quad (27)$$

If K_{eq} and the initial concentrations are known, z can be found by successive iteration of Equation 27.

As was done for the second oleum region, provision has been made to consider recombination of NO_2^+ and HSO_4^- via Equation 25. If this option is chosen in the model, Equations 23 and 25a must be solved simultaneously to give the equilibrium concentrations of the various ionic species. A procedure analogous to that used in the weak acid region to solve Equations 12d and 12e is employed.

Now, knowing initial concentrations, and having solved for the appropriate concentrations at equilibrium, Bennett's proposed rate expression can be applied to strong acid nitration as follows:

$$\frac{d[N]}{dt} = (k^I [HSO_4^-] + k^{II} [H_2SO_4] + k^{III} [HS_2O_7^-]) [M] [HNO_3]_0 Q \quad (28)$$

where Q is the fraction of nitric acid existing as nitronium ions;

$[M]$ is the concentration of nitrotoluene reactant;

$[N]$ is the concentration of nitrotoluene product; and

k^I , k^{II} , and k^{III} are rate constants.

It is emphasized that Equation 28 is continuous over the four strong acid regions previously described.

The influence of temperature upon reaction rate is taken into account by assuming, as Bennett did, that the constants k' , k'' , and k''' exhibit an Arrhenius dependence.

Thus, Equation 28 can be rewritten as:

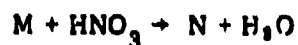
$$\frac{d[N]}{dt} = k_N \cdot \frac{-E_N}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right) (k_a [HSO_4^-] + k_b [H_2SO_4] + k_c [HS_2O_7^-]) [M] [HNO_3]_0 Q \quad (29)$$

and Equation 29 can be further simplified,

$$\text{Rate}_N = k_N \cdot \frac{-E_N}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right) [M] \gamma \quad (30)$$

$$\gamma = V_a (k_a [HSO_4^-] + k_b [H_2SO_4] + k_c [HS_2O_7^-]) [HNO_3]_0 Q \quad (31)$$

where k_N and E_N are the velocity coefficient and activation energy associated with the nitration reaction:



and V_a is the volume of the acid phase.

Subsequent to Bennett's work, strong experimental evidence was uncovered which contradicted a portion of his basic hypothesis. Melander demonstrated that proton departure from the transition compound during nitration is kinetically insignificant (Ref 12). Therefore, Bennett's contention that DNT nitration in mixed acid is a termolecular process dependent on both the nitronium ion and the proton acceptor ions, is most likely incorrect. In addition, for two-phase nitration systems, no maximum in

the rate at 92% H_2SO_4 has been noted.

Returning to Equations 16 and 17, it appears that there is sufficient justification to eliminate the proton acceptor component concentration terms from the expression for k_2 so that

$$k_2 = k \frac{[NO_2^+]}{[HNO_3]} \quad \text{and} \quad (31a)$$

$$\gamma = V_a k_2 [HNO_3] \quad (31b)$$

with the dependence of nitration on the concentrations of SO_3 , H_2SO_4 , and H_2O considered only in so far as those concentrations affect nitronium ion equilibria.

Although the nitration section simulation has been modified to utilize this simpler strong acid nitration model, the option to use Bennett's mechanism has been retained.

Far less is known about the kinetic mechanisms that govern the oxidation reactions which always occur to some extent during TNT manufacture along with the desired nitration reactions. With regard to oxidation, three key assumptions are made in the model: (1) oxidation reactions occur exclusively in the acid phase and therefore compete with the nitration reactions, (2) the controlling component in oxidation is the same as that which governs nitration (NO_2 ion), and (3) oxidation reactions exhibit bimolecular kinetics and are thus subject to the same reaction mechanisms as nitration. Also, because of a lack of plant data on cresol formation, oxidation of MNT is not represented in the model. This however, is not a critical shortcoming since cresols are eventually destructively oxidized to gaseous products and their contribution to overall yield loss can be compensated for by adjustment of the DNT oxidation rates. Equations A-42 through A-55 are employed in the model to represent oxidation.

Diffusion

Diffusion, as employed in the nitration section model, is the process by which the nitrobody components move between the two phases after their acid phase saturation solubility has been reached. This phenomenon depends solely upon the concentration gradients of the nitrobody species

across each phase and on the fluid properties of the medium as reflected by the mass transfer coefficient.

At steady state, diffusion of components toward the acid/organic interface must be equal to that away from it.

Thus,

$$D_i = \eta_{\phi} (y_i - y_i^*) = \eta_A (x_i^* - x_i) \quad (32)$$

where

$$x_i = \frac{A_i}{A_T} \quad \text{and} \quad y_i = \frac{\phi_i}{\phi_T} \approx \frac{\phi_i}{\phi_{nb}} \quad (33)$$

(See Figure 8 for an explanation of the nomenclature.)

Now, if we assume that the acid phase is always saturated with nitrobody,

$$A_{nb} = x_{eq}^A A_T \quad (34)$$

$$A_T = \frac{A_{NB}}{x_{eq}^A} \quad (35)$$

so that by substitution of Equation 35 into Equation 33 we get

$$x_i = \frac{A_i}{A_{nb}} x_{eq}^A \quad (36)$$

At the interface, the two phases must be in equilibrium. The equilibrium relationship assumed to be in effect is that the mole fraction nitrobody component in the organic phase must be equal to the acid-free mole fraction of that component in the acid phase.

Thus, at the interface,

$$\frac{\varphi_1^*}{\varphi_{nb}^*} = \frac{A_1^*}{A_{nb}^*} \quad (37)$$

but $A_{nb}^* = X_{eq}^A A_T^*$

so that
$$\frac{\varphi_1^*}{\varphi_{nb}^*} = \frac{A_1^*}{X_{eq}^A A_T^*} \quad (38)$$

or
$$y_1^* = x_1^*/X_{eq}^A \quad (39)$$

Substitution of the expressions for y_1 and y_1^* into Equation 32 gives

$$D_1 = \eta_\varphi \left(\frac{\varphi_1}{\varphi_{nb}} - \frac{x_1^*}{X_{eq}^A} \right) \quad (40)$$

but also from Equation 32,

$$x_1^* = \frac{D_1}{\eta_A} + x_1 \quad (41)$$

so that

$$D_1 = \eta_\varphi \left[\frac{\varphi_1}{\varphi_{nb}} - \frac{\left(\frac{D_1}{\eta_A} + x_1 \right)}{X_{eq}^A} \right] \quad (42)$$

$$D_1 = \eta_{\phi} \left(\frac{\varphi_1}{\varphi_{nb}} - \frac{D_1}{\eta_A X_{eq}^A} - \frac{x_1}{X_{eq}^A} \right) \quad (43)$$

$$\frac{D_1}{\eta_{\phi}} + \frac{D_1}{\eta_A X_{eq}^A} = \left(\frac{\varphi_1}{\varphi_{nb}} - \frac{x_1}{X_{eq}^A} \right) = \left(\frac{\varphi_1}{\varphi_{nb}} - \frac{A_1}{A_T X_{eq}^A} \right) \quad (44)$$

$$D_1 \left(\frac{1}{\eta_{\phi}} + \frac{1}{\eta_A X_{eq}^A} \right) = \frac{\varphi_1}{\varphi_{nb}} - \frac{A_1}{A_{nb}} \quad (45)$$

Now let

$$\frac{1}{\eta} = \left(\frac{1}{\eta_{\phi}} + \frac{1}{\eta_A X_{eq}^A} \right) \quad (46)$$

so that

$$D_1 = \eta \left(\frac{\varphi_1}{\varphi_{nb}} - \frac{A_1}{A_{nb}} \right) \quad (47)$$

Equation 47 is true for all organic components except toluene. For toluene, the reaction to MNT is so fast that it is assumed to occur at the interface, which eliminates the acid phase diffusion of toluene and forces A_{Tol} to be zero. Also the extremely rapid movement of toluene to the inter face warrants a separate mass transfer coefficient. Thus,

$$D_{Tol} = \eta_{Tol} \frac{\varphi_{Tol}}{\varphi_{nb}} \quad (48)$$

As indicated previously, the rate of conversion of toluene to MNT via Reactions 1 and 2 is solely dependent upon the rate of toluene diffusion so that

$$R_1 + R_2 = D_{Tol}$$

$$\frac{R_1}{R_2} = \frac{D_{Tol}}{R_2} - 1 \quad (49)$$

However, the ratio of aMNT to mMNT produced is dependent on the kinetic expressions:

$$\frac{aMNT}{mMNT} = \frac{R_1}{R_2} = \frac{k_1 \cdot e^{-\frac{E_1}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)}}{k_2 \cdot e^{-\frac{E_2}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)}} \quad (50)$$

$$\frac{R_1}{R_2} = \left(\frac{k_1}{k_2} \right) \cdot e^{\left[-\frac{E_1}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right) + \frac{E_2}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right) \right]} \quad (51)$$

$$\frac{R_1}{R_2} = \left(\frac{k_1}{k_2} \right) \cdot e^{-\frac{(E_1 - E_2)}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)} \quad (52)$$

$$\frac{R_1}{R_2} = k_{12} \cdot e^{-\frac{(E_1 - E_2)}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)} \quad (53)$$

Substitution of Equation 49 into Equation 53 gives

$$\frac{D_{Tol}}{R_1} - 1 = k_{12} e^{-\frac{(E_1 - E_2)}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)} \quad (54)$$

$$\frac{1}{R_1} = \frac{1 + k_{12} e^{-\frac{(E_1 - E_2)}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)}}{D_{Tol}} \quad (55)$$

Now, since $k_{12} e^{-\frac{(E_1 - E_2)}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)} \gg 1$, we can re-write Equation 55 as

$$R_1 = \frac{D_{Tol}}{k_{12} e^{-\frac{(E_1 - E_2)}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right)}} \quad (56)$$

$$R_1 = \frac{D_{Tol}}{k_{12}} e^{(E_1 - E_2)/R \left(\frac{1}{T} - \frac{1}{T_R} \right)} = \frac{D_{Tol}}{k_{12}} e^{(E_2 - E_1)/R \left(\frac{1}{T} - \frac{1}{T_R} \right)} \quad (57)$$

At this point, it should also be noted that while chemical reactions occur in both the nitrators and separators due to the ever present solubilized organic components in the acid phase, diffusion is assumed to be nonexistent in the separators because of the drastic reduction in inter-face area which occurs there.

Bulk Mass Transfer and Solubility

The remaining generation terms in the material balance equations (Equations 5 and 8) are those for bulk mass transfer. Bulk mass transfer, is in effect, the means by which equilibrium nitrobody solubility is enforced on the acid phase. At any point in the nitration section, the equilibrium amount of nitrobody in the acid phase is given by

$$A_{nb} = X_{eq}^A A_T \quad (58)$$

where X_{eq}^A has a value dependent on the local temperature as well as the local acid phase composition. For a given vessel, nitrobody is present in the acid phase by virtue of that which entered with the incoming acid phase, A_{nb}^O , that which diffused in from the organic phase, $\sum_{i=nb} D_i$, and that which resulted from a change in solubility created by combination of various vessel input streams which are obviously not in equilibrium. The last of these is considered the bulk mass transfer. Thus, to enforce equilibrium on the acid phase leaving the vessel, it must be true that

$$X_{eq}^A A_T = A_{nb}^O + \sum_{i=nb} D_i + M_{nb} \quad (59)$$

and

$$M_{nb} = X_{eq}^A A_T - A_{nb}^O - \sum_{i=nb} D_i \quad (60)$$

where M_{nb} represents the bulk movement of nitrobody into the acid phase which must occur in order to maintain equilibrium solubility. Negative values of M_{nb} are reasonable and indicate nitrobody dropping out of solution at the new vessel conditions. The individual component bulk mass transfer rates are computed from the overall bulk nitrobody transfer rate as follows:

$$M_i = \begin{cases} \frac{A_i}{A_{nb}} M_{nb} & \text{if } M_{nb} < 0 \\ \frac{\phi_i}{\phi_{nb}} M_{nb} & \text{if } M_{nb} \geq 0 \end{cases}$$

where the index i represents each nitrobody component. The change in acid phase nitrobody composition due to reaction is not included in the bulk mass transfer term since reaction only converts one nitrobody component to another and does not result in a net molar change.

An expression for the equilibrium solubility of bulk nitrobody in the acid phase has been developed by subjecting a limited quantity of published solubility data to a multiple regression procedure.* Solubility is correlated against temperature and acid phase composition to give:

$$x_{eq}^A = 10^p \quad (81)$$

where

$$p = 3.82 + .01023T - 3.808 x_{H_2O} + 7.716 x_{MNT} - 8.452 x_{TNT} - 6.292 x_{HNO_3} \quad (82)$$

*Laboratory solubility data for TNT, DNT, and MNT in mixed acid at various temperatures is currently being generated. This data, being more extensive than what is used for the existing solubility correlation, will be regressed to generate a new nitrobody solubility expression which is expected to significantly improve the nitration section model.

where

T is temperature in $^{\circ}\text{K}$

$x_{\text{H}_2\text{O}}$ is mole fraction water in acid phase

x_{MNT} is mole fraction MNT in acid phase

x_{TNT} is mole fraction TNT in acid phase

x_{HNO_3} is mole fraction nitric acid in acid phase

Finally, an expression has been developed to represent the solubility of nitric acid in the organic phase. It is the only acid component that shows any appreciable solubility in the organic phase. The expression used in the model is:

$$y_{\text{HNO}_3} = 1.51 x_{\text{H}_2\text{O}} \left(\frac{x_{\text{HNO}_3}}{x_{\text{H}_2\text{SO}_4}} \right) \quad (63)$$

Expressions for all of the terms in the vessel material balance equations (Equations 5 and 6) have now been developed so that if all vessel inputs are known and can be divided into acid and organic phase components, simultaneous solution of the vessel equations will give the output of that vessel in terms of moles per hour each component in each phase.

The vessel equations can be solved either for the transient state, in which case integration of the first order ordinary differential equations is required, or for the steady state, in which case the derivative terms are set equal to zero, resulting in a system of non-linear, simultaneous, coupled, algebraic equations. Both of these cases have been solved and the solution procedures including the computer programs generated will be described in detail in subsequent sections of this report.

Formulation of the Overall Nitration Section Model from the Single Vessel Model

Up to this point, discussion has centered around the details of the single vessel model without any regard to the way in which the complete 14-vessel nitration train (8 nitrators and 6 separators) is actually simulated. "Connection" of the individual vessels in the nitration section is

made possible by use of a physical separation model which takes the ideally separated organic and acid phases computed by the separator vessel model and constructs the three real streams which actually flow to other vessels. These include the organic stream forward to the next nitrator, the internal acid recycle stream, and the external acid recycle stream to the previous nitration stage. Because the separation process is not ideal, a portion of the acid phase is entrained in the organic stream leaving the separator and similarly, a portion of the organic phase is entrained in the two exiting acid streams.

In developing the equations for the physical separation model, the entrainments are defined as follows:

e_{oa} = molar fraction of the acid recycle stream, both internal and external, which is entrained organic phase.

e_{ao} = molar fraction of the organic stream which is entrained acid phase.

The following assumptions are also made: (1) the composition of entrained material is the same as that of the bulk phase from which it originated, (2) the composition of the internal and external recycle streams are identical, and (3) the values for e_{oa} and e_{ao} are constant for a given separator.*

The separation process is described schematically in Figure 9. It is again stressed that this physical separation model operates on the contents of a separator after the kinetic and mass transfer processes in that separator have transpired.

*An option exists in the model whereby e_{oa} and e_{ao} can be computed based on correlations that were developed using linear multiple regression techniques. However, because of the relatively high standard error of estimate associated with the correlation coefficients, e_{oa} and e_{ao} are usually assigned their constant values.

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Now, let

A_1 = moles/hr of acid phase in Stream 1

φ_1 = moles/hr of organic phase in Stream 1

Note that the flow rates A_0 and φ_0 of the acid and organic phases in the input stream are known.

First consider the separation of Stream 0 into Streams 1 and 2. From the definition of e_{oa} and e_{ao} :

$$e_{oa} = \frac{\varphi_1}{A_1 + \varphi_1} \quad (64)$$

$$e_{oa} = \frac{A_2}{A_2 + \varphi_2} \quad (65)$$

These can be converted into molar ratios as follows:

$$e_{oa}' = \frac{\varphi_1}{A_1} = \frac{e_{oa}}{1 - e_{ao}} = \text{molar ratio of organic phase to acid phase in recycle streams.} \quad (66)$$

$$e_{oa}' = \frac{A_2}{\varphi_2} = \frac{e_{ao}}{1 - e_{ao}} = \text{molar ratio of acid phase to organic phase in organic stream.} \quad (67)$$

Material balances around node A yield:

$$\varphi_0 = \varphi_1 + \varphi_2 \quad (68)$$

$$A_0 = A_1 + A_2 \quad (69)$$

Substituting Equation 66 for φ_1 and Equation 67 for A_2 gives:

$$\varphi_o = A_1 e'_{oa} + \varphi_2 \quad (70)$$

$$A_o = A_1 + \varphi_2 e'_{oa} \quad (71)$$

Eliminating φ_2 and rearranging, gives

$$f_{ar} = \frac{A_1}{A_o} = \frac{1 - e'_{ao} \varphi_o / A_o}{1 - e'_{ao} e'_{oa}} = \text{fraction of the entering acid phase that appears in the acid recycle stream.} \quad (72)$$

Solving Equation 70 for φ_2 , substituting Equation 72, and rearranging gives:

$$f_{po} = \frac{\varphi_2}{\varphi_o} = 1 - f_{ar} e'_{oa} A_o / \varphi_o \quad (73)$$

From f_{po} and f_{ar} the composition of each component in the organic stream can readily be calculated. Let A_{1j} be the moles/hr of Component j in the acid phase of Stream 1. Define φ_{1j} analogously to be the moles/hr of Component j in the organic phase of Stream 1. For Stream 2, these can be computed as follows:

$$A_{2j} = (1 - f_{ar}) A_{oj} \quad (74)$$

$$\varphi_{2j} = f_{po} \varphi_{oj} \quad (75)$$

Stream 1 must now be separated into its internal and external recycle portions. The volumes of the entering phases (Stream 0)

can be computed from their compositions:

$$Q_{\phi 0} = \text{ft}^3/\text{hr of organic phase in Stream 0}$$

$$Q_{A0} = \text{ft}^3/\text{hr of acid phase in Stream 0}$$

$$Q_{T0} = Q_{\phi 0} + Q_{A0} = \text{total ft}^3/\text{hr for Stream 0.}$$

The total flow of Stream 1 can be computed as:

$$Q_{T1} = f_{ar} Q_{A0} + (1-f_{po}) Q_{\phi 0} \quad (76)$$

The fraction of Stream 1 that appears in Stream 3 (internal acid recycle) is:

$$f_{ir} = \frac{Q_{T3}}{Q_{T1}} = \frac{Q_{max} f(N)}{f_{ar} Q_{A0} + (1-f_{po}) Q_{\phi 0}} \quad (77)$$

where Q_{max} = maximum ft^3/hr of internal recycle (a known constant) ,

N = notch setting on a gate valve in the internal recycle line which is modeled as an equal percentage valve ,

$f(N)$ = fraction of maximum flow corresponding to the notch setting .

The flow rates of the individual components in each phase of Streams 3 and 4 can be computed as follows:

$$A_{3j} = f_{ir} f_{ar} A_{0j} \quad (78)$$

$$\phi_{3j} = f_{ir} (1-f_{po}) \phi_{0j} \quad (79)$$

$$A_{4j} = (1-f_{ir}) f_{ar} A_{0j} \quad (80)$$

$$\phi_{4j} = (1-f_{ir}) (1-f_{po}) \phi_{0j} \quad (81)$$

Thus it is seen that the composition of the separator outlet streams can be calculated by the physical separation model from the results of the separator vessel model and that this in turn forms the basis for connection of the six nitration stages. The way in which the stages are connected will become clearer in the next section of the report, which deals with the implementation of the vessel and physical separation models on a digital computer to form the complete nitration section simulation.

COMPUTER IMPLEMENTATION OF THE MATHEMATICAL MODEL - THE SIMULATION

Separate computer programs have been prepared to simulate both the dynamic and steady states of the nitration process. While differing in solution procedure, there is no difference in their basic structures; both are ways to solve the vessel equations to give vessel outputs for known inputs. In fact, the solution obtained by running the dynamic simulation long enough to reach steady state is exactly that obtained by executing the steady state simulation, within the limits of numerical accuracy. A complete list of the vessel equations (the mathematical model of any nitration section vessel) ordered according to a logical solution sequence is given in Appendix A.

The Dynamic Simulation

The dynamic simulation is a computer program which, for a given set of nitration section independent variables including (1) feed rates (lb/hr), (2) composition of raw materials (wt%), (3) nitrator temperatures ($^{\circ}\text{C}$), and (4) recycle notch settings, will operate upon the vessel and physical separation equations to give the composition and flow rate (moles/hr) of the exiting streams from each of the 14 process vessels as functions of time. A numerical integration technique known as Euler's Method is employed to solve the differential equations. Although this is the simplest of the many numerical integration algorithms available, its efficiency in solving the vessel equations is satisfactory.

Formulation of the Equations

In order to solve the unsteady state vessel equations via Euler's Method, it is first necessary to reformulate the continuous differential equations (Equations 5 and 6) into their discrete numerical equivalents.

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For Component 1 (α MNT)*, Equation 5 is

$$A_{n,1}^O + R_{n,1}^A - R_{n,1}^O + D_{n,1} + M_{n,1} - A_{n,1} = \frac{d A_{n,1}}{dt} \quad (82)$$

and Equation 6 is

$$P_{n,1}^O - D_{n,1} - M_{n,1} - P_{n,1} = \frac{d P_{n,1}}{dt} \quad (83)$$

Equations 82 and 83 are not exactly correct since the units of all terms on the left side are moles/hr while those on the right are moles/hr³. To correct for this, the derivatives are rewritten as:

$$\frac{d}{dt} (V_n f_A \rho_A x_{n,1}) \text{ for } \frac{d A_{n,1}}{dt}$$

and

$$\frac{d}{dt} (V_n (1-f_A) \rho_P y_{n,1}) \text{ for } \frac{d P_{n,1}}{dt}$$

where

V_n is the vessel volume (ft³)

f_A is the volume fraction acid phase in the vessel

ρ_A is the density of the acid phase (moles/ft³)

ρ_P is the density of the organic phase (moles/ft³)

x_1 is the mole fraction of α MNT in the acid phase

y_1 is the mole fraction of α MNT in the organic phase.

Therefore Equations 82 and 83 can be rewritten as:

$$A_O + R_1 - R_2 + D_1 + M_1 - A_1 = \frac{d}{dt} (V f_A \rho_A x_1) \approx \frac{V f_A \rho_A}{A_T} \frac{d A_1}{dt} \quad (84)$$

* See Appendix A for component number assignments

$$P_0 - D_1 - M_1 - P_1 = \frac{d}{dt} [V(1-f_A) \rho_P y_1] = \frac{V(1-f_A) \rho_0}{A_T} \frac{dP_1}{dt} \quad (85)$$

Note that in Equations 84 and 85 the vessel subscripts have been dropped and the assumption that fraction acid, density, and total moles change little with time has been made.

The numerical approximations for the continuous derivatives are:

$$\frac{d A_1}{dt} = \frac{A_1^{t+\Delta t} - A_1^t}{\Delta t} \quad (86a)$$

$$\frac{d P_1}{dt} = \frac{P_1^{t+\Delta t} - P_1^t}{\Delta t} \quad (86b)$$

where the superscript t represents a quantity evaluated at the current time and $t+\Delta t$ indicated computation at the end of a time step. Substitution into Equations 84 and 85 yields:

$$[A_1^0 + R_1 - R_2 + D_1 + M_1 - A_1]^t = \frac{V f_A \rho_A}{A_T \Delta t} [A_1^{t+\Delta t} - A_1^t] \quad (87)$$

$$[P_1^0 - D_1 - M_1 - P_1]^t = \frac{V(1-f_A) \rho_P}{P_T \Delta t} [P_1^{t+\Delta t} - P_1^t] \quad (88)$$

Solving for $A_1^{t+\Delta t}$ and $P_1^{t+\Delta t}$ we get:

$$A_1^{t+\Delta t} = A_1^t + [A_1^0 + (R_1 - R_2) + D_1 + M_1 - A_1]^t \Delta t_A \quad (89)$$

$$P_1^{t+\Delta t} = P_1^t + [P_1^0 - D_1 - M_1 - P_1]^t \Delta t_P \quad (90)$$

where

$$\Delta t_A = \frac{A_T \Delta t}{V f_A \rho_A} \quad (\text{dimensionless})$$

$$\Delta t_P = \frac{P_T \Delta t}{V (1-f_A) \rho_P} \quad (\text{dimensionless})$$

Equations analogous to 88 and 90 may now be written for all components in the organic phase (except P_1 which is given by Equation 83) and for all components in the acid phase, and then solved via the Euler algorithm. This procedure was incorporated into the original computer program which was written to solve the unsteady state equations. Although the procedure is theoretically and numerically consistent, it was found that because of the large numerical values of the diffusion terms, a very small integration step size (Δt) was required in order to obtain numerical stability and generate convergent solutions. This was not acceptable, since use of an extremely small Δt resulted in intolerably long computer runs. To avoid this difficulty, an alternate solution procedure was devised based on the fact that the accumulation of nitrobody in the acid phase is small compared to that in the organic phase. This allows the integration of the nitrobody components to be carried out over the combined total amount of nitrobody in both phases, while the integration of the acid components in the acid phase is conducted as before. The concentration of the individual nitrobody components in the acid phase can then be obtained by solving the appropriate steady state equations after the integration has been carried out. In effect, it is assumed that the nitrobody in the acid phase is in equilibrium with that in the organic phase. Implementation of the procedure described above is carried out by first adding Equations 84 and 85 to give:

$$P_1^0 + A_1^0 + R_1 - R_2 = (P_1 + A_1) = \frac{V(1-f_A)\rho_P}{P_T} \frac{dP_1}{dt} + \frac{Vf_A\rho_A}{A_T} \frac{dA_1}{dt} \quad (91)$$

(Note that the troublesome mass transfer terms have dropped out of Equation 91.)

Now, let the total nitrobody in both phases be given by:

$$T_1 = P_1 + A_1 \quad (92)$$

so that

$$P_1 = T_1 - A_1 \quad (93)$$

Substitution of Equations 92 and 93 into Equation 91 yields:

$$P_1^0 + A_1^0 + R_1 - R_2 - T_1 = \frac{V(1-f_A)\rho_P}{P_T} \frac{dT_1}{dt} - \frac{V(1-f_A)\rho_P}{P_T} \frac{dA_1}{dt} + \frac{Vf_A\rho_A}{A_T} \frac{dA_1}{dt} \quad (94)$$

$$P_1^0 + A_1^0 + R_1 - R_2 - T_1 = \frac{V(1-f_A)\rho_P}{P_T} \frac{dT_1}{dt} + \left[\frac{Vf_A\rho_A}{A_T} - \frac{V(1-f_A)\rho_P}{P_T} \right] \frac{dA_1}{dt} \quad (95)$$

Since $\frac{dA_1}{dt} \ll \frac{dT_1}{dt}$

we can write:

$$P_1^0 + A_1^0 + R_1 - R_2 - T_1 \approx \frac{V(1-f_A)\rho_P}{P_T} \frac{dT_1}{dt} \quad (96)$$

In terms of discrete quantities:

$$T_1^{t+\Delta t} = T_1^t + \Delta t_P [P_1^0 + A_1^0 + R_1 - R_2 - T_1]^t \quad (97)$$

Equation 97 is called the normal or forward difference form of the discrete equation, where the term in brackets is evaluated at the beginning of the interval. However, the efficiency and stability of the numerical integration procedure is enhanced if the backward difference form is used, in which case the bracketed term is evaluated at the end of the interval. In this case:

$$T_1^{t+\Delta t} = T_1^t + \Delta t_P [P_1^0 + A_1^0 + R_1 - R_2 - T_1]^{t+\Delta t} \quad (98)$$

Solving for $T_1^{t+\Delta t}$, we get:

$$T_1^{t+\Delta t} = \frac{T_1^t + \Delta t_P [P_1^0 + A_1^0 + R_1 - R_2]^{t+\Delta t}}{1 + \Delta t_P} \quad (99)$$

But (from Appendix A),

$$R_2 = A_1 (G_{28} \delta + G_{28} \gamma) = A_1 F_2 \quad (100)$$

From the steady state equation

$$A_1^0 + R_1 - R_2 + D_1 + M_1 = A_1 = 0 \quad (101)$$

we can determine a value for A_1 as follows:

$$A_1 = A_1^0 + R_1 - G_{28} \delta A_1 - G_{28} \gamma A_1 + \eta \left(\frac{P_1}{P_{nb}} - \frac{A_1}{A_{nb}} \right) + M_{nb} \left(\frac{P_1}{P_{NB}} + \frac{A_1}{A_{nb}} \right) \quad (102)$$

$$\left(1 + G_{28} \delta + G_{28} \gamma + \frac{\eta}{A_{nb}} - \frac{M_{nb}}{A_{nb}} \right) A_1 = A_1^0 + R_1 + P_1 \left(\frac{\eta}{P_{nb}} + \frac{M_{nb}}{P_{nb}} \right) \quad (103)$$

But $P_1 = T_1 - A_1$ so that

$$\begin{aligned} & \left(1 + G_s \delta + G_{ss} \gamma + \frac{\eta}{A_{nb}} - \frac{M_{nb}}{A_{nb}}\right) A_1 = A_1^0 + R_1 \\ & + T_1 \left(\frac{\eta}{P_{nb}} + \frac{M_{nb}}{P_{nb}}\right) - A_1 \left(\frac{\eta}{P_{nb}} + \frac{M_{nb}}{P_{nb}}\right) \end{aligned} \quad (104)$$

$$\begin{aligned} & \left(1 + G_s \delta + G_{ss} \gamma + \frac{\eta}{A_{nb}} - \frac{M_{nb}}{A_{nb}} + \frac{\eta}{P_{nb}} + \frac{M_{nb}}{P_{nb}}\right) A_1 = A_1^0 \\ & + R_1 + T_1 \left(\frac{\eta}{P_{nb}} + \frac{M_{nb}}{P_{nb}}\right) \end{aligned} \quad (105)$$

$$A_1 = \frac{A_1^0 + R_1 + T_1 \left(\frac{\eta}{P_{nb}} + \frac{M_{nb}}{P_{nb}}\right)}{\left(1 + G_s \delta + G_{ss} \gamma + \frac{\eta}{A_{nb}} - \frac{M_{nb}}{A_{nb}} + \frac{\eta}{P_{nb}} + \frac{M_{nb}}{P_{nb}}\right)} \quad (106)$$

$$A_1 = \frac{A_1^0 + R_1 + T_1 (C_x)}{F_s + C_x} \quad (107)$$

where:

$$C_x = (\eta/P_{nb} + M_{nb}/P_{nb})$$

$$C_x = (1 + \eta/A_{nb} - M_{nb}/A_{nb} + C_x)$$

$$F_s = G_s \delta + G_{ss} \gamma$$

Substitution of Equations 100 and 107 into Equation 99 gives:

$$T_1^{t+\Delta t} = \frac{T_1^t + \Delta t_P [A_1^0 + P_1^0 + R_1 - \frac{F_1}{F_1 + C_2} (A_1^0 + R_1 + C_X T_1^{t+\Delta t})]^{t+\Delta t}}{1 + \Delta t_P} \quad (108)$$

Rearrangement of Equation 108 yields:

$$T_1^{t+\Delta t} = \frac{T_1^t + \Delta t_P X}{1 + \Delta t_P Y} \quad (109)$$

where

$$X = \left[P_1^0 + (R_1 + A_1^0) \left(1 - \frac{F_1}{F_1 + C_2} \right) \right] \quad (110)$$

$$Y = \left[1 + \left(\frac{F_1}{F_1 + C_2} \right) C_X \right] \quad (111)$$

The value of $A_1^{t+\Delta t}$ can now be computed from Equation 107 using the value of T determined in Equation 109. A_{nb}^t , M_{nb}^t , γ , and δ in Equation 107 are computed using the values of A_1^t and P_1^t rather than $A_1^{t+\Delta t}$ and $P_1^{t+\Delta t}$, but this has not posed any problems in the execution of the program. Equations similar to 109 can now be written to determine $T_2^{t+\Delta t}$ through $T_8^{t+\Delta t}$ with $A_2^{t+\Delta t}$ through $A_8^{t+\Delta t}$ being calculated from equations analogous to 107.

For the acid components in the acid phase, forward difference integration is employed.

$$\begin{aligned} A_9^{t+\Delta t} = & A_9^t + [A_9^0 + P_9^0 - P_9 - R_1 - R_2 - R_3 - R_4 - R_5 - R_6 \\ & - 13 R_7 - 12.5 R_8 - 9 R_{10} - 12.5 R_{10G} + (.33 + .67 RP) R_9 \\ & - A_9]^t \Delta t_A \end{aligned} \quad (112)$$

$$AL^{t+\Delta t} = AL^t + [A_{13}^0 - A_{14}^0 + R_1 + R_2 + R_3 + R_4 + R_5 + R_6$$

$$+ 15 R_7 + 18.5 R_8 + 12 R_{10} + 18.5 R_{10G} - (.33 RP + .87) R_9$$

$$- AL]^t \Delta t_A \quad (113)$$

$$\text{where } AL^{t+\Delta t} = A_{13}^{t+\Delta t} - A_{14}^{t+\Delta t} \quad (114)$$

$$\text{If } AL < 0$$

$$A_{13} = 0$$

$$A_{14} = AL$$

$$\text{and if } AL \geq 0$$

$$A_{13} = AL$$

$$A_{14} = 0$$

$$A_{13}^{t+\Delta t} = A_{13}^t + [A_{13}^0 + (11 R_7 + 14.5 R_8 + 9 R_{10} + 14.5 R_{10G}) (1-FD)$$

$$- A_{13}]^t \Delta t_A \quad (115)$$

$$A_{SO}^{t+\Delta t} = A_{SO}^t + [A_{11}^0 + A_{14}^0 - (11 R_7 + 14.5 R_8 + 9 R_{10}$$

$$+ 14.5 R_{10G}) (1-F_D) - A_{SO}]^t \Delta t_A \quad (116)$$

$$A_{11}^{t+\Delta t} = A_{SO}^{t+\Delta t} - A_{14}^{t+\Delta t} \quad (117)$$

Solution Procedure for Dynamic Simulation

The primary sequence of operations which must be executed in order to obtain the unsteady state solution of the nitration section equations is as follows:

Step 1: Enter the initial steady state of the process. This includes the composition and flow rates of the ideally separated acid and organic phases from each of the 14 process vessels, as well as the corresponding feed rates, compositions, nitrator temperatures, and notch settings.

Step 2: Process the initial conditions through the physical separation equations for all six separators to get initial conditions on the recycle streams.

Step 3: Read in the perturbations to the independent variables which constitute the deviations from steady state.

Step 4: Begin execution of the vessel equations for Vessel 1 (Nitrator 1A) by making up the terms required to compute the generation expressions D_1 , M_1 , and R_1 .

Step 5: Integrate using Equations 107 to 117 to get the values of P_1 and A_1 at the end of the first time step.

Step 6: Store these values as the current outputs from Nitrator 1A, and use them to make up the inputs to Nitrator 1B.

Step 7: Repeat Steps 4 and 5 for Nitrator 1B.

Step 8: Store these values as the current outputs from Nitrator 1B and use them to make up the inputs to Separator 1.

Step 9: Repeat Steps 4 and 5 for Separator 1.

Step 10: Store these values as the current ideally separated outputs from Separator 1.

Step 11: Process the current values of the ideally separated output from Separator 1 through the physical separation equations to give the current composition and flow of the three streams leaving Separator 1.

Step 12: Store these values for use in making up inputs to other vessels.

Step 13: Begin execution of vessel equations for Nitrator 2 and continue the procedure for all remaining vessels through Separator 6.

At this point, one complete pass will have been made across the entire nitration reactor train for the first time step with the values of each vessel's output used to make up the necessary inputs for execution during the second time step. This procedure is now repeated for n time steps as desired. The program currently employs a time step of .01 hours (36 seconds). Thus, to simulate 12 hours of process operation, 1200 time steps must be executed. Typically, the execution time required for such a case is about 120 seconds on the CDC 6500 computer giving an average of 0.1 second of machine time per time step.

Program Description

The nitration section dynamic simulation consists of a main program, four subroutine subprograms, and one function subprogram. Appendix B presents a complete program listing; Appendix C shows the program flow chart; Appendix D gives the program nomenclature; and Appendix E presents the input data format.

All programs are written in FORTRAN IV for compilation on the CDC FORTRAN extended (FTN) compiler, version 3.0 and require 65K (octal) words on the CDC 6500 computer for complete execution. Word length on the CDC 6500 is 60 bits. Since there are no machine-dependent routines, the program should execute on any comparable computer with only minor modifications. It should be noted that a number of library subroutines (NANCY, NUCAR, and NANCYM) are used to plot desired output.

The MAIN program reads in all data and parameter values, monitors and controls the sequential execution of the vessel and physical separation equations, and keeps track of all vessel inputs and outputs. The program also computes the values of a number of process performance indicators from the current values the vessel outflows at various times during the run and plots them as a function of time. These performance indicators constitute the primary output of the dynamic simulation and include: concentration of DNT in the crude TNT (wt %), flow rate of crude TNT (lb/hr); concentration of nitrobody in the spent acid (wt %), the fraction DNT in the spent acid nitrobody (wt %), concentration of water in the spent

acid (wt %), flow rate of spent acid (lb/hr), total carbon and nitrogen oxides in the off-gas (lb-moles/hr), heat loads in each nitrator (BTU/hr), concentration of nitric acid in the external recycle from each separator (wt % actual nitric), ratio of nitric to sulfuric acid in each nitrator, the amount of nitration occurring in each nitrator, and the specific gravities of the external acid recycle and organic streams leaving each separator. The values of e'_{oa} and e'_{oa} for each separator given by Equations 86 and 87 are also computed in the main program for later use in the physical separation equations.

Subroutine INPUT is called by the main program to read in the starting values of the independent variables including raw material feed rates and compositions, nitrator temperatures, and internal recycle notch setting, as well as to read in the magnitude and time of the desired perturbations to these quantities. Since feed rate data is entered in lb/hr, the subroutine makes the appropriate conversions to molar units. Also, the exponential factors in the rate equations (e.g.,

$$K_1 \exp \left[- \frac{F_1}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right) \right]$$

are precomputed in INPUT in order to increase the efficiency with which the vessel equations are executed.

The heart of the dynamic simulation is subroutine SUB. Here, all of the vessel and physical separation equations are executed and integrated each time the subroutine is called by the main program as it steps through the reactor train. In effect, the main program provides the necessary input data to SUB (i.e. the main program tells SUB whether it is a nitrator or separator and then which one it is in the reactor train; it provides vessel constants for that vessel such as volume and notch setting; it provides the input and output phase compositions for the vessel from the previous time step). SUB then generates the output of the vessel and returns. SUB also computes a temperature rise for each separator based on the adiabatic heat generated by the small amount of reaction which takes place there.

Subroutine SUB1 computes the change in the calculated values of the phase compositions for each vessel from one iteration to the next. An iteration is defined as the execution of m time steps where m is specified at the beginning of the run. SUB1 also flags that component in each vessel which shows the maximum change between iterations.

Subroutine SUB2 executes the physical separation equations for each separator using the steady state phase compositions of the input data. SUB2 is called by the main program prior to execution of the first time step only in order to initialize the recycle flows. The physical separation equations are thereafter executed in subroutine SUB as the run progresses.

The final subprogram in the dynamic simulation is function ENTH. This function is used in conjunction with the nitrator heat balance calculations executed by the main program. Its purpose is to calculate the enthalpy of any specified flow stream in the process by interpolating enthalpy-composition data which exists as a data table within the function. The enthalpies of the input and output streams are combined with the heats of reaction and heats of mixing to compute each nitrator's heat duty.

The Steady State Simulation

The steady state simulation is a computer program which, for a given set of nitration section independent variables, will execute the vessel and physical separation equations to give the steady state values of the composition and flow rates (moles/hr) of the exiting streams from each of the 14 process vessels. In addition, the values of a number of process performance functions are computed.

At steady state, the accumulation terms in Equations A-57 to A-82 go to zero so that differential equation system of the dynamic case becomes one of simultaneous algebraic equations. Because of the implicit nature of these equations, and also because of the presence of numerous recycle streams, a multilevel (nested) iteration procedure is used along with a simultaneous equation solving technique to arrive at the final solution.

Formulation of Equations

For the nitrobody components in the acid phase, the following system of steady state equations can be written:

$$\text{For component 1: } A_1^0 - R_1 + D_1 + M_1 - A_1 = 0 \quad (118)$$

$$A_1 + R_1 - D_1 - M_1 = A_1^0 \quad (119)$$

Substitution of Equations 18, 20, 21, and 38 from Appendix A into Equation 119 gives

$$A_1 + (G_s \delta + G_s S \gamma) A_1 - \eta \left(\frac{P_1}{P_{nb}} - \frac{A_1}{A_{nb}} \right) - M_{nb} \frac{A_1}{A_{nb}} - M_{nb} \frac{P_1}{P_{nb}} = A_1^0 \quad (120)$$

Simplifying,

$$A_1 (1 + G_s \delta + G_s S \gamma) - C_1 \left(\frac{P_1}{P_{nb}} - \frac{A_1}{A_{nb}} \right) - C_A A_1 - C_R P_1 = A_1^0 \quad (121)$$

where: $C_1 = \eta$

$$C_A = \frac{M_{nb}}{A_{nb}} \text{ for } M_{nb} < 0 \quad C_A = 0 \text{ for } M_{nb} \geq 0$$

$$C_R = \frac{M_{nb}}{P_{nb}} \text{ for } M_{nb} \geq 0 \quad C_R = 0 \text{ for } M_{nb} < 0$$

Further rearrangement of Equation 121 yields:

$$(1 + G_s \delta + G_s S \gamma + \frac{C_1}{A_{nb}} - C_A) A_1 - \left(\frac{C_1}{P_{nb}} + C_R \right) P_1 = A_1^0 \quad (122)$$

Similarly, for component 2:

$$A_2^0 - R_4 + D_2 + M_2 - A_2 = 0 \quad (123)$$

$$A_2 + R_4 - D_2 - M_2 = A_2^0 \quad (124)$$

Appropriate substitution from Appendix A yields:

$$A_2 + (G_4\delta + G_4S\gamma) A_2 - \frac{C_1}{P_{nb}} P_2 + \frac{C_1}{A_{nb}} A_2 - C_A A_2 - C_R P_2 = A_2^0 \quad (125)$$

$$A_2 (1 + G_4\delta + G_4S\gamma + \frac{C_1}{A_{nb}} - C_A) - (\frac{C_1}{P_{nb}} + C_R) P_2 = A_2^0 \quad (126)$$

For component 3:

$$A_3 + R_3 - R_3 - R_{1A} - R_{2A} - R_{3A} + D_3 + M_3 - A_3 = 0 \quad (127)$$

$$A_3 - R_3 + R_3 + R_{1A} - R_{2A} + R_{3A} - D_3 - M_3 = A_3^0 \quad (128)$$

$$A_3 - (G_3\delta + G_3S\gamma) A_1 + G_3\gamma A_3 + G_7\gamma A_3 + \frac{VG_3f_A A_3}{Q_A^1} A_3 + G_3\gamma A_3 - \frac{C_1}{P_{NB}} P_3 + \frac{C_1}{A_{NB}} A_3 - C_A A_3 - C_R P_3 = A_3^0 \quad (129)$$

$$A_3 \left(1 + G_3\gamma + G_7\gamma + \frac{VG_3f_A A_3}{Q_A^1} + G_3\gamma + \frac{C_1}{A_{nb}} - C_A \right) - \left(\frac{C_1}{P_{nb}} + C_R \right) P_3 = A_3^0 + (G_3\delta + G_3S\gamma) A_1 \quad (130)$$

For component 4:

$$A_4^0 + R_4 - R_4 - R_{1M} - R_{2M} - R_{3M} + D_4 + M_4 - A_4 = 0 \quad (131)$$

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$$A_4 - R_4 + R_6 + R_7 M + R_8 M + R_9 M - D_4 - M_4 = A_4^0 \quad (132)$$

$$A_4 - (G_4 \delta + G_{4S} \gamma) A_2 + G_4 \gamma A_4 + \frac{VG_4 f_A A_9}{Q_A^3} A_4 + G_4 \gamma A_4 - \frac{C_1}{P_{nb}} P_4 + \frac{C_1}{A_{nb}} A_4 - C_A A_4 - C_R P_4 = A_4^0 \quad (133)$$

$$A_4 \left(1 + G_4 \gamma + G_4 \gamma + \frac{VG_4 f_A A_9}{Q_A^3} + G_4 \gamma + \frac{C_1}{A_{nb}} - C_A \right) - \left(\frac{C_1}{P_{nb}} + C_R \right) P_4 = A_4^0 + (G_4 \delta + G_{4S} \gamma) A_2 \quad (134)$$

For component 5:

$$A_5^0 + R_5 - R_{10} A + D_5 + M_5 - A_5 = 0 \quad (135)$$

$$A_5 - R_5 + R_{10} A - D_5 - M_5 = A_5^0 \quad (136)$$

$$A_5 - G_5 \gamma A_5 + \frac{VG_{10} f_A A_{17}}{Q_A^3} A_5 - \frac{C_1}{P_{nb}} P_5 + \frac{C_1}{A_{nb}} A_5 - C_A A_5 - C_R P_5 = A_5^0 \quad (137)$$

$$A_5 \left(1 + \frac{VG_{10} f_A A_{17}}{Q_A^3} + \frac{C_1}{A_{nb}} - C_A \right) - \left(\frac{C_1}{P_{nb}} + C_R \right) P_5 = A_5^0 - G_5 \gamma A_5 \quad (138)$$

For component 6:

$$A_6^0 + R_6 - R_{10}M + D_6 + M_6 - A_6 = 0 \quad (139)$$

$$A_6 - R_6 + R_{10}M - D_6 - M_6 = A_6^0 \quad (140)$$

$$A_6 - G_6 \gamma A_6 + \frac{VG_{10} f_A A_{17}}{Q_A} A_6 - \frac{C_1}{P_{nb}} P_6 + \frac{C_1}{A_{nb}} A_6 - C_A A_6 - C_R P_6 = A_6^0 \quad (141)$$

$$A_6 \left(1 + \frac{VG_{10} f_A A_{17}}{Q_A} + \frac{C_1}{A_{nb}} - C_A \right) - \left(\frac{C_1}{P_{nb}} + C_R \right) P_6 = A_6^0 + G_6 \gamma A_6 \quad (142)$$

For component 7:

$$A_7^0 + R_{10} + D_7 + M_7 - A_7 = 0 \quad (143)$$

$$A_7 - R_{10} - D_7 - M_7 = A_7^0 \quad (144)$$

$$A_7 - \frac{VG_{10} f_A A_{17}}{Q_A} (A_6 + A_6) - \frac{C_1}{P_{nb}} P_7 + \frac{C_1}{A_{nb}} A_7 - C_A A_7 - C_R P_7 = A_7^0 \quad (145)$$

$$A_7 \left(1 + \frac{C_1}{A_{nb}} - C_A \right) - \left(\frac{C_1}{P_{nb}} + C_R \right) P_7 = A_7^0 + \frac{VG_{10} f_A A_{17}}{Q_A} (A_6 + A_6) \quad (146)$$

For component 8:

$$A_8^0 + 3 R_{18} + D_8 + M_8 - A_8 = 0 \quad (147)$$

$$A_8 - 3 R_{18} - D_8 - M_8 = A_8^0 \quad (148)$$

$$A_8 - \frac{3VG_{18}f_A A_{17}}{Q_A^*} (A_8 + A_8) - \frac{C_1}{P_{nb}} P_8 + \frac{C_1}{A_{nb}} A_8 - C_A A_8 - C_R P_8 = A_8^0 \quad (149)$$

$$A_8 \left(1 + \frac{C_1}{A_{nb}} - C_A \right) - \left(\frac{C_1}{P_{nb}} + C_R \right) P_8 = A_8^0 + \frac{3VG_{18}f_A A_{17}}{Q_A^*} (A_8 + A_8) \quad (150)$$

For the nitrobody species in the organic phase, the steady state vessel equations can be written as follows:

$$P_1^0 + R_1 - M_1 - D_1 - P_1 = 0 \quad (151)$$

$$P_1 - R_1 + M_1 + D_1 = P_1^0 \quad (152)$$

$$P_1 - D_{18} (1 - G_1) + C_A A_1 + C_R P_1 + \frac{C_1}{P_{nb}} P_1 - \frac{C_1}{A_{nb}} A_1 = P_1^0 \quad (153)$$

$$\text{but } D_{18} = \eta_{\text{Tol}} \frac{P_{18}}{P_{nb}} = C_1' P_{18} \quad (154)$$

so that,

$$P_1 - C_1' P_{10} (1 - G_1) + A_1 \left(C_A - \frac{C_1}{A_{nb}} \right) + P_1 \left(C_R + \frac{C_1}{P_{nb}} \right) = P_1^0 \quad (155)$$

$$\begin{aligned} \left(C_A - \frac{C_1}{A_{nb}} \right) A_1 + \left(1 + C_R + \frac{C_1}{P_{nb}} \right) P_1 &= P_1^0 \\ &+ C_1' P_{10} (1 - G_1) \end{aligned} \quad (156)$$

For component 2:

$$P_1^0 + R_1 - M_1 - D_1 - P_1 = 0 \quad (157)$$

$$P_1 - R_1 + M_1 + D_1 = P_1^0 \quad (158)$$

$$P_1 - C_1' P_{10} G_1 + C_A A_1 + C_R P_1 + \frac{C_1}{P_{nb}} P_1 - \frac{C_1}{A_{nb}} A_1 = P_1^0 \quad (159)$$

$$\left(C_A - \frac{C_1}{A_{nb}} \right) A_1 + \left(1 + C_R + \frac{C_1}{P_{nb}} \right) P_1 = P_1^0 + C_1' P_{10} G_1 \quad (160)$$

For component 3:

$$P_1^0 - M_1 - D_1 - P_1 = 0 \quad (161)$$

$$P_1 + M_1 + D_1 = P_1^0 \quad (162)$$

$$P_1 + C_A A_1 + C_R P_1 + \frac{C_1}{P_{nb}} P_1 - \frac{C_1}{A_{nb}} A_1 = P_1^0 \quad (163)$$

$$(C_A - \frac{C_1}{A_{nb}}) A_3 + (1 + C_R + \frac{C_1}{P_{nb}}) P_3 = P_3^0 \quad (164)$$

For component 4:

$$P_4^0 - M_4 - D_4 - P_4 = 0 \quad (165)$$

$$P_4 + M_4 + D_4 = P_4^0 \quad (166)$$

$$(C_A - \frac{C_1}{A_{nb}}) A_4 + (1 + C_R + \frac{C_1}{P_{nb}}) P_4 = P_4^0 \quad (167)$$

Similarly, for components 5 through 8:

$$C_{21} A_5 + C_{22} P_5 = P_5^0 \quad (168)$$

$$C_{21} A_6 + C_{22} P_6 = P_6^0 \quad (169)$$

$$C_{21} A_7 + C_{22} P_7 = P_7^0 \quad (170)$$

$$C_{21} A_8 + C_{22} P_8 = P_8^0 \quad (171)$$

where:

$$C_{21} = C_A - \frac{C_1}{A_{nb}} \text{ and } C_{22} = (1 + C_R + \frac{C_1}{P_{nb}})$$

Now, for toluene:

$$P_{10}^0 - D_{10} P_{10} = 0 \quad (172)$$

$$P_{10} + D_{10} = P_{10}^0 \quad (173)$$

$$P_{10} (1 + C_1') = P_{10}^0 \quad (174)$$

$$P_{10} = P_{10}^0 / (1 + C_1') \quad (175)$$

For the acid species in the acid phase, the steady state vessel equations are written as follows:

$$A_0^0 + P_0^0 - P_0 - D_{10} - R_2 - R_4 - R_5 - R_6 - 13R_7 - 12.5R_8 - 9R_{10} - 12.5R_9G + (.33 + .67RP) R_9 - A_0 = 0 \quad (176)$$

Making the appropriate substitutions from Appendix A gives:

$$\begin{aligned} & A_0 + P_0 + C_1 P_{10} + (G_2\delta + G_2s\gamma) A_1 + (G_4\delta + G_4s\gamma) A_2 + G_5\gamma A_3 \\ & + G_6\gamma A_4 + 13G_7\gamma (A_3 + A_4) + 12.5 \left(\frac{VG_8f_A}{Q_A} [HNO_3] \right) (A_3 + A_4) \\ & + 12.5G_9\gamma (A_3 + A_4) + 9 \left(\frac{VG_{10}f_A}{Q_A} [NO_3^+] \right) (A_3 + A_4) \\ & - (.33 + .67RP) F_D C_0 = A_0^0 + P_0^0 \\ & A_0 + P_0 + C_1 P_{10} + F_2 A_1 - F_4 A_2 + \left(G_5\gamma + 13G_7\gamma + 12.5 \frac{VG_8f_A}{Q_A} [HNO_3] \right. \\ & \left. + 12.5G_9\gamma \right) A_3 + \left(G_6\gamma + 13G_7\gamma + 12.5 \frac{VG_8f_A}{Q_A} [HNO_3] + 12.5G_9\gamma \right) A_4 \\ & + 9 \frac{VG_{10}f_A}{Q_A} [NO_3^+] A_3 + 9 \frac{VG_{10}f_A}{Q_A} [NO_3^+] A_4 - (.33 + .67RP) F_D C_0 \\ & = A_0^0 + P_0^0 \end{aligned} \quad (177)$$

$$\text{Also, } P_9 = \left(\frac{1.51 A_{13} P_T}{A_T A_{11}} \right) A_9 \quad (178)$$

$$A_{11}^O + A_{14}^O - C_9 P - A_{SO_4} = 0 \quad (179)$$

$$A_{SO_4} + (1 - F_D) C_9 = A_{11}^O + A_{14}^O \quad (180)$$

$$A_{11}^O + C_9 P - A_{13} = 0 \quad (181)$$

$$A_{13} - C_9 P = A_{11}^O \quad (182)$$

$$\begin{aligned} A_{13}^O - A_{14}^O + R_1 + R_2 + R_3 + R_4 + R_5 + R_6 + 15R_7 + 16.5R_8 + 12R_{10} \\ + 16.5R_{10} - (.33R_P + .67)R_9 - A_L = 0 \end{aligned} \quad (183)$$

$$\begin{aligned} A_L - C_1 P_{10} - F_3 A_1 - F_4 A_2 - \left(G_6 \gamma + 15G_7 + 16.5 \frac{VG_8 f_A}{Q_A} [\text{HNO}_3] \right. \\ \left. + 16.5G_9 \gamma \right) A_3 - \left(G_6 \gamma + 15G_7 \gamma + 16.5 \frac{VG_8 f_A}{Q_A} [\text{HNO}_3] \right. \\ \left. + 16.5G_9 \gamma \right) A_4 - 12 \frac{VG_{10} f_A}{Q_A} [\text{NO}_3^+] A_5 - 12 \frac{VG_{10} f_A}{Q_A} [\text{NO}_3^+] A_6 \\ \left. + (.33RP + .67) F_D C_9 = A_{11}^O + A_{14}^O \right) \quad (184) \end{aligned}$$

Equations 122, 126, 130, 134, 138, 142, 146, 150, 156, 160, 164, 167, 168, 169, 170, 171, 175, 177, 178, 179, 182, and 184 are linear in the following unknowns: A_1 through A_9 , A_{SO_4} , A_{11} , A_L , and P_1 through P_{10} . This

constitutes a system of 22 equations and 22 unknowns which is solvable provided the coefficients of all the unknown terms can be determined.

Solution Procedure for the Steady State Simulation

Execution of the steady state simulation consists mainly of the simultaneous solution of the 22 vessel equations for each of the 14 vessels in the nitration train. Although these equations could be solved simultaneously via Gauss reduction, it was decided that because of the sparsity of the coefficient matrix, a straightforward direct substitution approach would be more efficient. This will become clear as the step-by-step solution procedure is outlined below. The physical separation equations must also be employed here as in the dynamic case to convert computed pure phase outputs to real stream outputs. As mentioned previously, a multilevel or nested iterative procedure is used because of (1) the implicit nature of the vessel equations (the coefficients of the linear unknowns are functions of these unknowns), and (2) the numerous recycle streams in the process.

The primary sequence of operations which must be executed in order to obtain the steady solution is as follows:

Step 1: Enter an assumed solution for the phase outputs from each of the 14 process vessels.

Step 2: Enter the values of the process's independent variables for which the steady state solution is desired.

Step 3: Using the assumed solution for the vessel phase outputs, compute the flow rates and compositions of all recycle streams in the process via the physical separation equations.

Step 4: Begin the iterative solution of the vessel equations for the first vessel (Nitrator #1A). Start by computing the values of all coefficients of the 22 x 22 vessel equation matrix from the assumed solution for that vessel. Also, make up the correct phase inputs to Nitrator 1A.

Step 5: Solve Equation 175 for P_{10} .

Step 6: Solve Equations 122 and 156 simultaneously for values of A_1 and F_1 .

Step 7: Solve Equations 126 and 160 simultaneously for values of A_1 and P_1 .

Step 8: Solve Equations 130 and 164 simultaneously for values of A_2 and P_2 .

Step 9: Solve Equations 134 and 167 simultaneously for values of A_3 and P_3 .

Step 10: Solve Equations 138 and 168 simultaneously for values of A_4 and P_4 .

Step 11: Solve Equations 142 and 169 simultaneously for values of A_5 and P_5 .

Step 12: Solve Equations 146 and 170 simultaneously for values of A_6 and P_6 .

Step 13: Solve Equations 150 and 171 simultaneously for values of A_7 and P_7 .

Step 14: Solve Equations 176 and 178 simultaneously for values of A_8 and P_8 .

Step 15: Solve Equation 182 for A_{11} .

Step 16: Solve Equation 184 for A_L .

Step 17: Use the logic of Equations A-70 and A-71 to determine values for A_{13} and A_{14} .

Step 18: If computed values and assumed values differ by more than a predetermined amount, repeat Steps 5 through 17 using newly computed values for the A_i 's and P_i 's.

Step 19: Repeat Step 18 until convergence is achieved on Nitrator 1A.

Step 20: Using the converged solution for Nitrator 1A, and the previously assumed recycle stream flows, make up the correct phase inputs to Nitrator 1B and then repeat Step 4 for Nitrator 1B.

Step 21: Repeat Steps 5 through 17 for Nitrator 1B.

Step 22: Repeat Step 18 for Nitrator 1B.

Step 23: Repeat Step 22 until convergence is achieved on Nitrator 1B.

Step 24: Using the converged solution for Nitrator 1B as the input to Separator 1 and the initially assumed phase outputs, execute Steps 4 through 19 for Separator 1.

Step 25: Process the converged outputs for Separator 1 through the physical separation equations to get the flow rates and compositions of the recycle streams leaving that separator.

Step 26: Compare the calculated recycle stream between Separator 1 and Nitrator 1B (internal recycle) to that assumed when the inputs to Nitrator 1B were made up. If they differ by a preset amount, use the newly calculated recycle stream, and the previously converged values of the outputs from Nitrators 1A and 1B to repeat Steps 4 through 19 for Nitrator 1B.

Step 27: Repeat Steps 24 through 26 until convergence on the internal recycle stream is achieved.

Step 28: Using the converged Separator 1 outputs and the originally assumed Nitrator 2 output and Separator 3 recycle stream values, execute Steps 4 through 19 for Nitrator 2.

Step 29: Repeat Steps 24 through 27 for Separator 2.

Step 30: Repeat Steps 28 and 29 for Stages 3 through 6 until convergence on all internal recycle streams is achieved. Note, although a converged solution for each stage will have been obtained at this point, no attempt at linking the six stages together through their external recycle streams has yet been made. This must now be done in order to obtain the complete steady state solution for the 14-vessel reactor train.

Step 31: Begin with the external recycle between Separator 6 and Nitrator 5. Using the previously converged outputs from Separators 4, 5, and 6 as Nitrator 5 inputs and the previously converged Nitrator 5 output, execute Steps 4 through 19 for Nitrator 5.

Step 32: Repeat Steps 24 through 27 for Separator 5.

Step 33: Execute Steps 4 through 19 for Nitrator 6 using the newly converged Separator 5 output and previously converged Separator 6 and Nitrator 6 outputs.

Step 34: Repeat Steps 24 through 27 for Separator 6.

Step 35: Compare the newly calculated external acid recycle stream from Separator 6 to that employed in Step 31. If they differ by a preset amount, use the newly calculated value as well as the most recently converged values for the other required flows to repeat Steps 31 through 34.

Step 36: Repeat Step 35 until convergence on the external recycle from Separator 6 is achieved.

Step 37: Continue with this stagewise iteration procedure until the remaining external recycle streams (and thus the entire nitration reactor train) have been converged.

Typically, a steady state run requires approximately 5000 iterations of the vessel equations with convergence limits set at .05 mole/hr for overall vessel composition, .02 moles/hr for components in the internal recycle, and .02 moles/hr for components in the external recycle. Under these conditions, program execution time is approximately 30 seconds on the CDC 6500. Obviously, if tighter convergence is desired, run time increases significantly.

Program Description

The nitration section steady state simulation consists of a main program, two subroutine subprograms, and one function subprogram. A complete steady state run including the program listing is presented in Appendix F. Appendix G shows the program flow chart; Appendix H gives the program nomenclature; and Appendix I illustrates the input data format.

All programs are written in FORTRAN IV for compilation on the CDC FORTRAN extended (FTN) compiler, version 3.0, and will compile and execute in 55,000 (octal) words on the CDC 6500. Since there are no machine-dependent routines, the program should execute on any comparable computer with only minor modifications. A brief description of the main program and the three subprograms will now be given.

The main program (TNTSIM) reads in all data and parameter values which form the fixed data base for the steady state simulation. Included in this data base is an initial guess at the steady state solution. Also, the program is responsible for reading the particular set of values for the independent process input variables for which the steady state output is desired. All feed streams which are entered as lb/hr are converted to moles/hr and the Arrhenius factors are precomputed for later use in the rate expressions as are values for e_{a0} and e_{oa} . However, the primary function of the main program is to monitor and control the execution of the three-level convergence procedure employed to arrive at the steady state solution. The program is actually responsible for external recycle convergence and calls the appropriate subroutines for internal recycle or vessel convergence. The program also assigns and updates vessel identification parameters so that it can correctly sequence through the reactor system. After overall convergence is achieved, the main program prints out the steady state values of the ideal phase and actual stream compositions and flow rates from each nitrator and separator in the process (including the off-gas streams) and then proceeds to compute and print out the values of a number of process performance indicators including vessel time constants (hours), overall molar yield, flow rate of crude TNT (lb/hr), DNT in the crude TNT (wt %), raw material cost (\$/lb TNT), spent acid flow (lb/hr) and composition, extent of nitration in each stage, acid composition in each stage (in units similar to those generated by plant operators during control checks), nitrobody density in each stage (lb/ft³), and heat duty in each nitrator. An elemental material balance is also run to check the consistency of the converged solution. The complete steady state printout is shown in Appendix F.

Subroutine NITSEP is employed to carry out the internal recycle convergence procedure. It is called by the main program during individual stage convergence and then again during total process convergence. The subroutine compares the current and previously computed values for the internal acid recycle leaving a given separator and does the required updating if the difference exceeds a predetermined value.

The heart of the steady state simulation program is subroutine VESSEL. Here, all of the vessel and physical separation equations are solved to give the output of each nitrator and separator during execution of the nested iteration convergence procedure. The subroutine is thus responsible for the execution and convergence of the primary iteration loop, i.e. the individual vessel. VESSEL is called by the main program and by subroutine NITSEP during the uncoupled stage convergence

procedure and then again by subroutine NITSEP during total process convergence. The calling program provides the necessary input data to VESSEL, such as whether it is to simulate a nitrator or a separator, the values of all input streams and the currently assumed output of the vessel. VESSEL will then execute Steps 4 through 19 of the solution procedure and, if the vessel has been flagged as a separator, process the converged vessel output through the physical separation equations. A modified direct substitution procedure is used, whereby a percentage of the difference between quantities calculated during successive iterations is added to the newly calculated quantity.

The final subprogram in the steady state simulation is function ENTH. It serves the same purpose here as it did in the dynamic simulation.

Parameter Fitting

As has been illustrated, the vessel equations are interspersed with a number of constants. These include terms associated with kinetic phenomena such as frequency factors, activation energies, and concentration exponents, as well as mass transfer coefficients, equilibrium constants, and solubility factors. In most cases, the appearance of these constants in the vessel equations is theoretically consistent and not simply a function of empirical supposition. An attempt was made to use published, experimentally determined values of constants when such values were available. However, because many needed values were simply not available, and, because most of those that were had been developed under laboratory conditions not comparable to the state of the actual nitration process, it was necessary to fit the constants (parameters) to steady state process operating data (steady state snapshots).

The parameter fitting procedure consisted of (1) assuming an initial value for each of the 27 parameters, (2) executing the steady state simulation with these parameter values and input variables values corresponding to specific data snapshots, (3) comparing computed outputs (molar component flows of all process streams) with observed snapshot values, and (4) making appropriate changes in parameter values to give better agreement between calculated and observed quantities.

A total of 14 steady state snapshots were available for parameter fitting. This data was obtained during normal operations at the production facility located at the Radford Army Ammunition Plant. A typical snapshot is shown in Table I of Appendix J. Of the 14 snapshots, seven were used for fitting with the remaining sets being employed to check the validity of the final fit.

In order to use the snapshot data (which is essentially stream compositions in weight %) for fitting purposes, it was first necessary to convert from units of composition to units of molar flow rate for each component. This was accomplished by processing the snapshot data through a material balance program, the details of which can be found in Reference 1. With the snapshot data in correct form for comparison with the individual stage outputs calculated by the simulation, it was simply required to make repetitive steady state runs and after each run, to evaluate an objective function. This function was in effect a measure of the total weight deviation from observed conditions in all nitration stages. Changes were then made to the parameter set which drove the objective function toward a minimum.

Minimization of the objective function was accomplished systematically by using a pattern search algorithm which was added to the steady state simulation as a subroutine and controlled program execution. The pattern search technique will be described in detail in the next section of the report when steady state optimization is discussed. A list of parameters with their final fit values is included in Table II of Appendix J.

APPLICATION OF THE SIMULATION

The computer simulation of the nitration section has been used to carry out a variety of studies on the nitration process. Most significant among these has been the use of the steady state simulation to develop optimized operating conditions and the development of a multivariable control procedure for vessel acid composition using the dynamic simulation to generate the process transfer function.

It is not intended that this report serve as the documentary record of the exploitation of the nitration section simulation. Detailed technical reports on specific studies using the nitration section simulation have been prepared (see Ref 15 to 17). However, it is desired in this volume to give the reader some feeling for the way in which the nitration section simulation can be used. With this in mind, the following description of two major areas of exploitation is presented.

Steady State Applications

Steady state optimization was carried out by making multiple steady state runs under the control of the same pattern search algorithm that was used during parameter fitting. The pattern search method is one of a number of direct climbing (Ref 13) techniques which will move toward an extremum of a multidimensional objective function based on previous information

about the response surface. The particular pattern search algorithm used was an adaptation of a procedure developed by Hooke and Jeeves (Ref 14) which employs accelerated climbing and has ridge-following properties.

For each steady state run made under control of the pattern search subroutine, an objective function, defined as the raw material cost per pound of TNT, was evaluated. The independent variables over which the search was made included feed composition, feed flow rate, nitrator temperature and internal recycle rate. The feed rate of toluene to the process (and therefore the production rate) was not varied during steady state optimization so that what was sought was the set of independent variables which gave the minimum raw material cost per pound of α -TNT produced at a fixed production rate. The fixed toluene rate employed during optimization was 2350 lb/hr, which corresponds to a TNT production rate of approximately 57 tons/day based on an 87% α -yield. The raw material cost per pound of TNT was calculated from the equation:

$$C = \frac{(Tx C_T) + (Sx C_S) + (Nx C_N) + (Wx C_W)}{(Tx Y)} \quad (185)$$

where:

C	= raw material cost (\$/lb TNT)
T	= toluene flow rate (lb/hr)
S	= oleum flow rate (lb/hr)
N	= strong nitric acid flow rate (lb/hr)
W	= weak nitric acid flow rate (lb/hr)
C _T	= cost of toluene (\$/lb toluene)
C _S	= cost of oleum (\$/lb)
C _N	= cost of strong nitric acid (98.5% HNO ₃) (\$/lb)
C _W	= cost of weak nitric acid (61.0% HNO ₃) (\$/lb)
Y	= yield (lb TNT/lb toluene)

Values of cost factor employed were based on data supplied by Radford Army Ammunition Plant and thus reflected that plant's raw material cost as of July 1972. Specific values used were: $C_T = .0293$, $C_S = .01182$, $C_W = .01061$, $C_N = .01714$.

Rather than consider all independent variables simultaneously, a sensitivity analysis was carried out which enabled ranking these variables in the order in which perturbations in them affected the objective function. Only main effect sensitivities were determined. Although the possibility of significant higher order effects could not be discounted, it was felt that the complexity of multiple-effect analysis (including increased machine time requirements) was not justified.

The independent variables were thus divided into five blocks according to their effects on the objective function, and pattern searches were conducted separately over each block. Since the number of variables per search was reduced by this procedure, the pattern search algorithm functioned more efficiently and saved computer time. The complete list of independent variables, ranked in decreasing order of their effects on the objective function and broken down into their search blocks, is shown in Table I of Appendix K.

Because of physical limitations in the actual process, a number of constraints on the independent variables had to be included in the objective function to insure that only feasible sets of process operating conditions were considered. This was accomplished by assigning penalty values to the objective function whenever a constraint value of one or more of the independent variables was under consideration of the search routine. This "brute force" method worked satisfactorily in keeping the search within feasible areas of the response surface. The constraints employed were based on information supplied by plant operating personnel at Radford and are listed in Table II of Appendix K.

As the optimization proceeded, it became evident that a substantial reduction in oleum was being made by the search program. Because of the magnitude of the predicted reduction (nearly 50% of the baseline feed rate), the validity of the model in a region so far from conditions under which parameters were fit came into question. Also, even if the simulation's predictions were correct, it was felt that plant operating personnel would never agree to such a drastic reduction in oleum flow. But the qualitative result was clear--cut back on oleum flow.

Consequently, the oleum flow rate was treated as a parameter, with sets of optimum conditions being developed for oleum flow rates of 11,000, 10,000, 9,000, 8,000, and 7,000 lb/hr. Of course, the lowest unit cost of TNT is predicted for the lowest oleum flow rate. Predicted optimum conditions for 10,000 lb/hr oleum are shown in Table K3 of Appendix K. For the interested reader, a more complete description of certain aspects of the steady state optimization studies can be found in Reference 3. In general, however, steady state optimization studies have resulted in the development of operating conditions which predict savings on the order of 20% in the raw material cost per pound of TNT.

Dynamic Applications

The primary application of the dynamic simulation has been its use in conjunction with the design of a supervisory control strategy for acid composition in each stage of nitration. The need to control the composition of the acid phase in each nitration stage is a result of the critical effect which this variable has on the extent of reaction. The object of the control study was thus to develop a procedure whereby predicted optimum acid concentrations could be maintained throughout the process in view of uncontrollable fluctuations in such things as raw material acid composition, internal flows, mixing characteristics, and heat transfer coefficients, as well as step changes in production rate.

It was determined that the way to accomplish this was to control specific indicators of acid concentration in all six external recycle streams and in the emulsion stream flowing from Nitrator 3A to Nitrator 3B by manipulating the seven primary nitric acid feeds and the yellow waterfeeds to the process. A system of nine manipulated and nine controlled variables results. The specific indicator of acid composition is optional and can be either total acidity, actual nitric acid, or nitric to sulfuric acid ratio. Control strategies employing various combinations of these controlled variables have been tested and shown to be feasible and the most promising approach appears to be control of total acidity and actual nitric acid in Stages 1 and 2 with the nitric to sulfuric ratio being controlled at the remaining five locations. Controlled variables with their proposed manipulated variables are listed in Figure 10.

The details of control strategy development have been documented elsewhere (Ref 15), although a number of significant points should be noted here. Because of the many recycle streams in the process, it was necessary

to develop a decoupling mechanism in order to counteract the disturbances created in adjacent nitrators when a feed change is made. Secondly, because of difficulties in obtaining real time measurements of the controlled variables, it was also necessary to develop a computational scheme to estimate the values of the desired controlled variables from measurable data and certain assumed constant values generated by the steady state program. A block diagram of the overall scheme for acid concentration control is shown in Figure 11. Note that the process simulation provides the necessary process dynamics in the same way, as an assumed transfer function (e.g., a first order lag plus dead time) would have, had not a detailed process model been used.

A number of runs were made with the simulated control scheme in order to develop reasonable values for controller tuning parameters. The open and closed loop responses of the system to a 10% step change in oleum flow are shown in Figures 12 and 13, respectively, for a typical run.

The dynamic simulation was also used in conjunction with a simulation of the nitrator temperature cascade control loop which is included in the software package provided by the Foxboro Company as part of the Volunteer AAP direct digital computer control system, scheduled to begin operation in late 1974. Performance of the temperature control system was tested for normal continuous operation on a single nitrator simulation and also for start-up operations on the complete six-stage nitration section simulation. The details and significant results of this effort can be found in Reference 16.

CONCLUSION

The modeling and simulation study of the continuous TNT process has resulted in much being learned about the chemical and physical phenomena which govern the process's behavior. Quantification of process interactions has made possible the generation of optimum operating conditions, improvements in the process design, and has allowed the development of a supervisory control strategy. Implementation of the results of the simulation effort is anticipated during calendar year 1974 when new computer-controlled TNT lines will be started up at Volunteer Army Ammunition Plant in Chattanooga, Tennessee. Only after verification of model predictions on the actual process and use of the model-developed process control strategies, will the full benefit of the simulation undertaking be realized. While simulation studies on other processes are planned, much will depend on the successful implementation of the TNT process simulation study's results.

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APPENDIX A
Vessel Equations

The following is an ordered set of equations which make up the kinetics and mass transfer model for any vessel in the nitration section of the continuous TNT process. The order in which they are listed represents the logical sequence of calculation employed in SUBROUTINE SUB of the dynamic simulation and SUBROUTINE VESSEL of the steady state simulation program.

Component Index Assignments

<u>Component</u>	<u>Index (i)</u>
α MNT	1
mMNT	2
α DNT	3
mDNT	4
α TNT	5
mTNT	6
TNB	7
TNBX	8
HNO ₃	9
Toluene	10
H ₂ SO ₄	11
HNOSO ₄	12
H ₂ O	13
SO ₃	14
Not used	15
Not used	16
NO ₂ ⁺	17

Equations

$$A_{NB} = \sum_{i=1}^8 A_i \quad (A-1)$$

$$P_{NB} = \sum_{i=1}^8 P_i + P_{10} \quad (A-2)$$

$$A_T = A_{NB} = A_0 + A_{11} + A_{12} + A_{13} + A_{14} \quad (A-3)$$

$$P_T = P_{NB} + P_9 \quad (A-4)$$

$$Q_A = \sum_{i=1}^{10} \frac{A_i}{P_i} \quad (A-5)$$

$$Q_P = \sum_{i=1}^{10} \frac{P_i}{P_i} \quad (A-6)$$

$$F_A = \frac{Q_A}{Q_A + Q_P} \quad (A-7)$$

$$F_P = 1 - F_A \quad (A-8)$$

$$\text{When vessel is a separator, } F_A = .755 \quad (A-8a)$$

$$X_1 = \frac{A_1}{A_T} \quad (A-9)$$

$$X_{eq}^A = 10^P \quad (A-10)$$

Where:

$$P = 3.62 + 0.01023 T - 3.808 X_{10} + 7.716 \quad (A-11)$$

$$(X_1 + X_2) - 8.452 (X_3 + X_4) - 6.292 X_5$$

$$\eta_A = VF_P \text{ kma} \quad (A-12)$$

$$\eta_P = VF_P (kma)_P \quad (A-13)$$

$$\eta_{Tol} = VF_P (kma)_{Tol} \quad (A-14)$$

$$\eta = \left(\frac{1}{\frac{1}{\eta_P} + \frac{1}{\eta_A X_{eq}^A}} \right) \quad (A-15)$$

$$D_i = \eta \left(\frac{P_i}{P_{NB}} - \frac{A_i}{A_{NB}} \right) \quad i = 1, 8 \quad (A-16)$$

$$D_{10} = \eta_{Tol} \left(\frac{P_{10}}{P_{NB}} \right) \quad (A-17)$$

$$A_{NB} = (X_{eq}^A) A_T \quad (A-18)$$

$$M_{NB} = A_{NB} - A_{NB}^O - \sum_{i=1}^8 D_i \quad (A-19)$$

$$\text{If } M_{NB} < 0: M_i = M_{NB} \left(\frac{A_i}{A_{NB}} \right) \quad i = 1, 8 \quad (A-20)$$

$$\text{If } M_{NB} \geq 0: M_i = M_{NB} \left(\frac{P_i}{P_{NB}} \right) \quad (A-21)$$

$$\gamma = \frac{VF_A}{Q_A} [NO_2^+] (k_a [HSO_4^-] + k_b [H_2SO_4] + k_c [HS_2O_7^-]) \quad (A-22)$$

or

$$\gamma = k_a \frac{Vf_A}{Q_A} [\text{NO}_2^+] \quad (\text{A-23})$$

All concentrations are equilibrium values resulting from dissociations according to the mechanisms outlined in Section V, Volume I of this report.

$$Z = -\frac{1}{R} \left(\frac{1}{T} - \frac{1}{T_R} \right) \quad (\text{A-24})$$

$$G_1 = \frac{1}{k_{1s}} \exp(E_{1s}Z) \quad (\text{A-25})$$

$$G_2 = k_{2w} \exp(E_{2w}Z) \quad (\text{A-26})$$

$$G_{2s} = k_{2s} \exp(E_{2w}Z) \quad (\text{A-27})$$

$$G_4 = k_{4w} \exp(E_{4w}Z) \quad (\text{A-28})$$

$$G_{4s} = k_{4s} \exp(E_{4s}Z) \quad (\text{A-29})$$

$$G_{5s} = k_{5s} \exp(E_{5s}Z) \quad (\text{A-30})$$

$$G_6 = k_{6s} \exp(E_{6s}Z) \quad (\text{A-31})$$

$$G_7 = k_7 \exp(E_7Z) \quad (\text{A-32})$$

$$G_8 = k_8 \exp(E_8Z) \quad (\text{A-33})$$

$$G_9 = k_9 \exp(E_9Z) \quad (\text{not used}) \quad (\text{A-34})$$

$$G_{10} = k_{10} \exp (E_{10} Z) \quad (A-35)$$

$$R_2 = D_{10} G_1 \quad (A-36)$$

$$R_1 = D_{10} - R_2 \quad (A-37)$$

$$R_3 = (G_3 \gamma) A_1 \quad (A-38)$$

$$R_4 = (G_4 \gamma) A_2 \quad (A-39)$$

$$R_5 = G_5 \gamma A_3 \quad (A-40)$$

$$R_6 = G_6 \gamma A \quad (A-41)$$

$$R_{7A} = G_7 \frac{Vf_A}{Q_A} [NO_2^+] A_3 ; R_{7M} = G_7 \frac{Vf_A}{Q_A} [NO_2^+] A_4 \quad (A-42)$$

$$R_7 = R_{7A} + R_{7M} \quad (A-43)$$

$$R_{8A} = \frac{VG_8 f_A}{Q_A} [NO_2^+] A_3 \quad (A-44)$$

$$R_{8M} = \frac{VG_8 f_A}{Q_A} [NO_2^+] A_4 \quad (A-45)$$

$$R_8 = R_{8A} + R_{8M} \quad (A-46)$$

$$R_{9A} = G_9 \gamma A_3 \quad (A-47)$$

$$R_{9M} = G_9 \gamma A_4 \quad (A-48)$$

$$R_{9G} = R_{9A} + R_{9M} \quad (A-49)$$

(not used)

U

$$R_{10A} = \frac{VG_{10}f_A}{Q_A} [\text{NO}_2^+] A_0 \quad (\text{A-50})$$

$$R_{10M} = \frac{VG_{10}f_A}{Q_A} [\text{NO}_2^+] A_0 \quad (\text{A-51})$$

$$R_{10} = R_{10A} + R_{10M} \quad (\text{A-52})$$

$$C_0 = 11R_7 + 14.5R_8 + 9R_{10} + 14.5R_{10G} \quad (\text{A-53})$$

$$R_9 = (F_D) (C_0) \quad (\text{A-54})$$

$$C_{sp} = C_0 - R_9 = C_0 (1-F_D) \quad (\text{A-55})$$

$$\tau_A = \frac{Vf_{ApA}}{A_T} \quad (\text{A-56})$$

$$A_1^0 = R_3 + D_1 + M_1 - A_1 = \tau_A \frac{dA_1}{dt} \quad (\text{A-57})$$

$$A_2^0 = R_4 + D_2 + M_2 - A_2 = \tau_A \frac{dA_2}{dt} \quad (\text{A-58})$$

$$\begin{aligned} A_3^0 + R_3 - R_6 - R_{7A} - R_{8A} - R_{9A} + D_3 + M_3 - A_3 \\ = \tau_A \frac{dA_3}{dt} \end{aligned} \quad (\text{A-59})$$

$$\begin{aligned} A_4^0 + R_4 - R_8 - R_{7M} - R_{8M} - R_{9M} + D_4 + M_4 - A_4 \\ = \tau_A \frac{dA_4}{dt} \end{aligned} \quad (\text{A-60})$$

$$A_8^0 + R_8 - R_{10}A + D_8 + M_8 - A_8 = \tau_A \frac{dA_8}{dt} \quad (A-81)$$

$$A_8^0 + R_8 - R_{10}M + D_8 + M_8 - A_8 = \tau_A \frac{dA_8}{dt} \quad (A-82)$$

$$A_7^0 + R_{10} + D_7 + M_7 - A_7 = \tau_A \frac{dA_7}{dt} \quad (A-83)$$

$$A_8^0 + 3R_{10} + D_8 + M_8 - A_8 = \tau_A \frac{dA_8}{dt} \quad (A-84)$$

$$A_9^0 + P_9^0 - P_9 - D_{10} - R_9 - R_4 - R_8 - R_6 - 13R_7 \\ - 12.5R_8 - 9R_{10} - 12.5R_{9G} + (.33 + .67 RP) R_9$$

$$- A_9 = \tau_A \frac{dA_9}{dt} \quad (A-85)$$

$$A_{10} = 0 \quad (A-86)$$

$$A_{11}^0 + A_{10}^0 - C_8P - A_{8O_4} = \tau_A \frac{dA_{8CA}}{dt} \quad (A-87)$$

$$A_{12}^0 + C_8P - A_{12} = \tau_A \frac{dA_{12}}{dt} \quad (A-88)$$

$$A_{10}^0 - A_{10}^0 + R_1 + R_2 + R_3 + R_4 + R_5 + R_6 + 15R_7 \\ + 16.5R_8 + 12R_{10} + 16.5R_{9G} - (.33R_P + .67) R_9$$

$$- A_L = \tau_A \frac{dA_L}{dt} \quad (A-89)$$

$$\text{If } A_L < 0 \quad (A-70)$$

$$A_{13} = 0$$

$$A_{14} = A_L$$

$$\text{If } A_L > 0 \quad (A-71)$$

$$A_{13} = A_L$$

$$A_{14} = 0$$

$$A_{11} = A_{SO_4} - A_{14} \quad (A-72)$$

$$r_P = \frac{V(1-f_A)}{P_T} \rho_P \quad (A-73)$$

$$P_1^0 + R_1 - M_1 - D_1 - P_1 = \frac{dP_1}{dt} \quad (A-74)$$

$$P_2^0 + R_2 - M_2 - D_2 - P_2 = r_P \frac{dP_2}{dt} \quad (A-75)$$

$$P_3^0 - M_3 - D_3 - P_3 = r_P \frac{dP_3}{dt} \quad (A-76)$$

$$P_4^0 - M_4 - D_4 - P_4 = r_P \frac{dP_4}{dt} \quad (A-77)$$

$$P_5 - M_5 - D_5 - P_5 = r_P \frac{dP_5}{dt} \quad (A-78)$$

$$P_1^0 - M_6 - D_6 - P_6 = r_P \frac{dP_6}{dt} \quad (A-79)$$

$$P_7^0 - M_7 - D_7 - P_7 = r_P \frac{dP_7}{dt} \quad (A-80)$$

$$P_0^0 - M_0 - D_0 - P_0 = \tau_P \frac{dP_0}{dt} \quad (A-81)$$

$$P_{10}^0 - D_{10} - P_{10} = \tau_P \frac{dP_{10}}{dt} \quad (A-82)$$

$$P_0 = 1.81 \left(\frac{A_{12} A_2}{A_{11}} \right) \left(\frac{P_T}{A_T} \right) \quad (A-83)$$

$$G_{CO_{1.8}} = R_{10} + 6R_7 + 7R_8 + 7R_9 G \quad (A-84)$$

$$G_{NO} = .67R_9 (1 - R_P) \quad (A-85)$$

$$G_{TNM} = R_7 \quad (A-86)$$



Appendix B
Dynamic Simulation--Program Listing and Output

[illegible]


```

345      M0TCH=N3
      FVCM=FVCM5
      ITYPE=1
      D06701=1.14
      A35(1)=A(1)
      P35(1)=P(1)
      A(1)=A35(1)
      P(1)=P35(1)
      A(1)=A35(1)
      P(1)=P35(1)
      PI(1)=PI(1)
      PI(1)=PI(1)
      CONTINUE
670      CALL SUB
      IF (J.NE.NN) GOT0671
      WRITE(6,507)
507      FORMAT(12HSEPARATOR 1)
      WRITE(6,401)
      CALL SUB(1A,P,A1,P1)
671      CONTINUE
      ITYPE=0
      FRAC=FRAC
      F2=1.-FRAC3
      F3=FRAC
      F03=FPO
      FAC(10)=1.-F03
      F06G=1.-F03
      ISTGE=4
      IV=6
      T=76
      FVCM=FVCM4
      D06801=1.14
      A35(1)=A(1)
      P35(1)=P(1)
      A(1)=A4(1)
      P(1)=P4(1)
      PI(1)=PI(1)
      PI(1)=A4(1)+FAC(10)*A3(1)+F06G*A55(1)+F03*
      PI(1)=F03+P35(1)+F06G*A55(1)+F06G
      IF (IQUIT.EQ.3) GOT03
      CALL SUB
      IF (J.NF.NN) GOT0681
      WRITE(6,509)
509      FORMAT(11HSEPARATOR 4)
      WRITE(6,401)
      CALL SUB(1A,P,A1,P1)
681      CONTINUE
      EOP=EOAP4
      EAP=EAOP4
      M0TCH=N4
      FVCM=FVCM5
      ITYPE=1
      D06901=1.14
      A4(1)=A(1)
      P4(1)=P(1)
      A(1)=A45(1)
      P(1)=P45(1)
      PI(1)=PI(1)
      PI(1)=A4(1)
      PI(1)=P4(1)
      CONTINUE
690

```

ADDRESS	INSTRUCTIONS	PC	PC+1	PC+2	PC+3	PC+4	PC+5	PC+6	PC+7	PC+8	PC+9	PC+10	PC+11	PC+12	PC+13	PC+14	PC+15	PC+16	PC+17	PC+18	PC+19	PC+20	PC+21	PC+22	PC+23	PC+24	PC+25	PC+26	PC+27	PC+28	PC+29	PC+30	PC+31	PC+32	PC+33	PC+34	PC+35	PC+36	PC+37	PC+38	PC+39	PC+40	PC+41	PC+42	PC+43	PC+44	PC+45	PC+46	PC+47	PC+48	PC+49	PC+50	PC+51	PC+52	PC+53	PC+54	PC+55	PC+56	PC+57	PC+58	PC+59	PC+60	PC+61	PC+62	PC+63	PC+64	PC+65	PC+66	PC+67	PC+68	PC+69	PC+70	PC+71	PC+72	PC+73	PC+74	PC+75	PC+76	PC+77	PC+78	PC+79	PC+80	PC+81	PC+82	PC+83	PC+84	PC+85	PC+86	PC+87	PC+88	PC+89	PC+90	PC+91	PC+92	PC+93	PC+94	PC+95	PC+96	PC+97	PC+98	PC+99	PC+100	PC+101	PC+102	PC+103	PC+104	PC+105	PC+106	PC+107	PC+108	PC+109	PC+110	PC+111	PC+112	PC+113	PC+114	PC+115	PC+116	PC+117	PC+118	PC+119	PC+120	PC+121	PC+122	PC+123	PC+124	PC+125	PC+126	PC+127	PC+128	PC+129	PC+130	PC+131	PC+132	PC+133	PC+134	PC+135	PC+136	PC+137	PC+138	PC+139	PC+140	PC+141	PC+142	PC+143	PC+144	PC+145	PC+146	PC+147	PC+148	PC+149	PC+150	PC+151	PC+152	PC+153	PC+154	PC+155	PC+156	PC+157	PC+158	PC+159	PC+160	PC+161	PC+162	PC+163	PC+164	PC+165	PC+166	PC+167	PC+168	PC+169	PC+170	PC+171	PC+172	PC+173	PC+174	PC+175	PC+176	PC+177	PC+178	PC+179	PC+180	PC+181	PC+182	PC+183	PC+184	PC+185	PC+186	PC+187	PC+188	PC+189	PC+190	PC+191	PC+192	PC+193	PC+194	PC+195	PC+196	PC+197	PC+198	PC+199	PC+200	PC+201	PC+202	PC+203	PC+204	PC+205	PC+206	PC+207	PC+208	PC+209	PC+210	PC+211	PC+212	PC+213	PC+214	PC+215	PC+216	PC+217	PC+218	PC+219	PC+220	PC+221	PC+222	PC+223	PC+224	PC+225	PC+226	PC+227	PC+228	PC+229	PC+230	PC+231	PC+232	PC+233	PC+234	PC+235	PC+236	PC+237	PC+238	PC+239	PC+240	PC+241	PC+242	PC+243	PC+244	PC+245	PC+246	PC+247	PC+248	PC+249	PC+250	PC+251	PC+252	PC+253	PC+254	PC+255	PC+256	PC+257	PC+258	PC+259	PC+260	PC+261	PC+262	PC+263	PC+264	PC+265	PC+266	PC+267	PC+268	PC+269	PC+270	PC+271	PC+272	PC+273	PC+274	PC+275	PC+276	PC+277	PC+278	PC+279	PC+280	PC+281	PC+282	PC+283	PC+284	PC+285	PC+286	PC+287	PC+288	PC+289	PC+290	PC+291	PC+292	PC+293	PC+294	PC+295	PC+296	PC+297	PC+298	PC+299	PC+300	PC+301	PC+302	PC+303	PC+304	PC+305	PC+306	PC+307	PC+308	PC+309	PC+310	PC+311	PC+312	PC+313	PC+314	PC+315	PC+316	PC+317	PC+318	PC+319	PC+320	PC+321	PC+322	PC+323	PC+324	PC+325	PC+326	PC+327	PC+328	PC+329	PC+330	PC+331	PC+332	PC+333	PC+334	PC+335	PC+336	PC+337	PC+338	PC+339	PC+340	PC+341	PC+342	PC+343	PC+344	PC+345	PC+346	PC+347	PC+348	PC+349	PC+350	PC+351	PC+352	PC+353	PC+354	PC+355	PC+356	PC+357	PC+358	PC+359	PC+360	PC+361	PC+362	PC+363	PC+364	PC+365	PC+366	PC+367	PC+368	PC+369	PC+370	PC+371	PC+372	PC+373	PC+374	PC+375	PC+376	PC+377	PC+378	PC+379
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13.13.61.

11/15/74

FTN 4.1-PSH367

PROGRAM THTSIM 74/74 OPT=1

```

460      FAS=FAR
      FOS=FPO
      FACIOS=1.-FAS
      FORGS=1.-FOS
      TSTGE=4
      IV=8
      VT=6
      FVTH=FVTHS
      D0720=1.14
      A55(1)=A(1)
      PSS(1)=P(1)
      A(1)=A6(1)
      P(1)=P6(1)
      A(1)=A5(1)+FACIOS*P5(1)+FRAC6*A6S(1)+FAS
      P(1)=FOS+PSS(1)+FRAC6*P6S(1)+FORG6
720      CONTINUE
      IF(TOUTT.EQ.5)GOTO3
      CALL SUB
      WRITE(6,512)
512      FORMAT(11M)ITRATOR 6)
      WRITE(6,401)
      CALL SUB(1A,P,AI,PI)
721      CONTINUE
      FOR=ECAP6
      EAP=EAP6
      NOTCH=6
      FVTH=FVTHS
      ITYPE=1
      D0730=1.14
      A6(1)=A(1)
      P6(1)=P(1)
      A(1)=A6S(1)
      P(1)=P6S(1)
      A(1)=A6(1)
      P(1)=P6(1)
730      CONTINUE
      CALL SUB
      FRAC6=FRAC
      FRC=1.-FRAC6
      FAS=FAR
      FOS=FPO
      FORGS=1.-FOS
      FACIO6=1.-FAS
      IF(IJ.NE.MN)GOTO731
      WRITE(6,513)
513      FORMAT(12M)SEPARATOR 4)
      WRITE(6,401)
      CALL SUB(1A,P,AI,PI)
      WRITE(6,247)CHARNIO,CHPMIO,DFANIO,DFPMIO
247      FORMAT(18M)CONVERGENCE TESTS./401.4MCI0.4X.8MORGANIC./
      1 50MAXIMUM PERCENT ERROR FROM STEADY STATE EQUATIONS.2F10.3/
      2 6XMAXIMUM PERCENT CHANGE FROM PREVIOUS ITERATION.3X.2F10.3)
      WRITE(6,246) (1.1=1.6).FACIO.FORG.FRC
246      FORMAT(48M)PARAMETERS USED IN RECYCLE CALCULATIONS/6X 50STAGE.
      C 271610/6X 3MFRACFACIO IN ORG. STREAM.6F8.5/
      C 6X 3MFRACFACIO IN ACID STREAM.6F8.5/

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11/15/74 13.13.41.

FTN 4.1-PS3367

PROGRAM THTSIN 74/74 OPT=1

THTDY 744

END

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
6153 THTSIN

VARIABLES	SN	TYPE	RELOCATION	406	AA	REAL	ARRAY	SEP	INPUT
0 A	0	REAL	ARRAY VECTOR	0	A1	REAL	ARRAY	SEP	20
442 AF	73	REAL	ARRAY	73	AK10	REAL	ARRAY	SEP	20
486 AJP	61	REAL	ARRAY	61	AK35	REAL	ARRAY	SEP	20
76 AKWATL	53	REAL	20	53	AK45	REAL	20	20	20
46 AK12	54	REAL	20	54	AK55	REAL	20	20	20
47 AK1M	51	REAL	20	51	AK7	REAL	20	20	20
50 AKON	57	REAL	20	57	AK9	REAL	20	20	20
52 AKOS	101	REAL	20	101	AK9	REAL	20	20	20
60 AKB	31447	REAL	ARRAY	31447	AK9	REAL	ARRAY	ARRAY	ARRAY
25323 AN	33647	REAL	ARRAY	33647	AK9	REAL	ARRAY	ARRAY	ARRAY
13465 ANAC	0	REAL	ARRAY	0	AKT	REAL	ARRAY	ARRAY	ARRAY
13466 ANAC	72	REAL	ARRAY	72	AKT	REAL	ARRAY	ARRAY	ARRAY
0 ABOAT	16256	REAL	ARRAY	16256	ATM	REAL	ARRAY	ARRAY	ARRAY
16250 ATM	16264	REAL	ARRAY	16264	AVL	REAL	ARRAY	ARRAY	ARRAY
0 AV	0	REAL	ARRAY	0	A1A	REAL	ARRAY	ARRAY	ARRAY
426 ATR	0	REAL	ARRAY	0	A1B	REAL	ARRAY	ARRAY	ARRAY
0 A1A1	21	REAL	ARRAY	21	A1B	REAL	ARRAY	ARRAY	ARRAY
21 A101	72	REAL	ARRAY	72	A15	REAL	ARRAY	ARRAY	ARRAY
42 A2	42	REAL	ARRAY	42	A21	REAL	ARRAY	ARRAY	ARRAY
115 A25	63	REAL	ARRAY	63	A3A	REAL	ARRAY	ARRAY	ARRAY
63 A3A1	104	REAL	ARRAY	104	A3R	REAL	ARRAY	ARRAY	ARRAY
104 A301	174	REAL	ARRAY	174	A35	REAL	ARRAY	ARRAY	ARRAY
125 A4	125	REAL	ARRAY	125	A41	REAL	ARRAY	ARRAY	ARRAY
155 A45	146	REAL	ARRAY	146	A45	REAL	ARRAY	ARRAY	ARRAY
146 A51	167	REAL	ARRAY	167	A61	REAL	ARRAY	ARRAY	ARRAY
167 A6	167	REAL	ARRAY	167	A61	REAL	ARRAY	ARRAY	ARRAY
217 A45	21011	REAL	ARRAY	21011	CDMT	REAL	ARRAY	ARRAY	ARRAY
22141 CMTSA	735	REAL	ARRAY	735	CHANGLO	REAL	ARRAY	ARRAY	ARRAY
737 CMTSNO	21445	REAL	ARRAY	21445	CHUSA	REAL	ARRAY	ARRAY	ARRAY
14 CP	21237	REAL	ARRAY	21237	CHUDE	REAL	ARRAY	ARRAY	ARRAY
21713 CUSA	36147	REAL	ARRAY	36147	CHMS	REAL	ARRAY	ARRAY	ARRAY
37753 CHUSA	734	REAL	ARRAY	734	CHMS	REAL	ARRAY	ARRAY	ARRAY
748 CHMSA	34	REAL	ARRAY	34	CHMS	REAL	ARRAY	ARRAY	ARRAY
13470 CHMS	1	REAL	ARRAY	1	CHMS	REAL	ARRAY	ARRAY	ARRAY
13473 CHMS	16242	REAL	ARRAY	16242	CHMS	REAL	ARRAY	ARRAY	ARRAY
26 FAOP	26	REAL	ARRAY	26	FAOP1	REAL	ARRAY	ARRAY	ARRAY
27 FAOP2	70	REAL	ARRAY	70	FAOP3	REAL	ARRAY	ARRAY	ARRAY
31 FAOP4	32	REAL	ARRAY	32	FAOP5	REAL	ARRAY	ARRAY	ARRAY
33 FAOP6	53	REAL	ARRAY	53	FAOP	REAL	ARRAY	ARRAY	ARRAY
11714 FFO	14234	REAL	ARRAY	14234	FOA	REAL	ARRAY	ARRAY	ARRAY
20 FOAP	20	REAL	ARRAY	20	FOAP1	REAL	ARRAY	ARRAY	ARRAY
21 FOAP2	22	REAL	ARRAY	22	FOAP3	REAL	ARRAY	ARRAY	ARRAY
23 FOAP	24	REAL	ARRAY	24	FOAP5	REAL	ARRAY	ARRAY	ARRAY
25 FOAP6	11716	REAL	ARRAY	11716	FOA	REAL	ARRAY	ARRAY	ARRAY
54 FOP	11713	REAL	ARRAY	11713	FOA	REAL	ARRAY	ARRAY	ARRAY
0 FX	11715	REAL	ARRAY	11715	FOA	REAL	ARRAY	ARRAY	ARRAY
71 F10	62	REAL	ARRAY	62	F21	REAL	ARRAY	ARRAY	ARRAY
55 F35	63	REAL	ARRAY	63	F3V	REAL	ARRAY	ARRAY	ARRAY
56 F45	64	REAL	ARRAY	64	F4V	REAL	ARRAY	ARRAY	ARRAY
65 F55	66	REAL	ARRAY	66	F65	REAL	ARRAY	ARRAY	ARRAY
67 F7	70	REAL	ARRAY	70	F8	REAL	ARRAY	ARRAY	ARRAY

11/15/76 13.13.01.

FTN 4.1058367

74/76 OPT=1

PROGRAM INTSTM

RELOCATION

SN TYPE

VARIABLES

211	P101	REAL	ARRAY	AMNT	240	P15	REAL	ARRAY	SEP
252	P2	REAL	ARRAY	AMNT	261	P25	REAL	ARRAY	SEP
273	P1A	REAL	ARRAY	AMNT	314	P30	REAL	ARRAY	AMNT
302	P75	REAL	ARRAY	SEP	375	P4	REAL	ARRAY	AMNT
323	P45	REAL	ARRAY	SEP	376	P5	REAL	ARRAY	AMNT
344	P55	REAL	ARRAY	SEP	377	P6	REAL	ARRAY	AMNT
365	P65	REAL	ARRAY	SEP	13467	0	REAL	ARRAY	AMNT
13471	04	REAL	ARRAY	SEP	22367	04	REAL	ARRAY	000
13463	0P	REAL	ARRAY	DUM	07	RATES	REAL	ARRAY	/ /
0	0	REAL	ARRAY	Z0	13	R001	REAL	ARRAY	Z0
11	R-010	REAL	ARRAY	Z0	12	R0011	REAL	ARRAY	Z0
13	R-012	REAL	ARRAY	Z0	14	R0013	REAL	ARRAY	Z0
15	R-014	REAL	ARRAY	Z0	1	R-02	REAL	ARRAY	Z0
2	R-023	REAL	ARRAY	Z0	3	R-04	REAL	ARRAY	Z0
4	R-025	REAL	ARRAY	Z0	5	R-046	REAL	ARRAY	Z0
6	R-027	REAL	ARRAY	Z0	7	R-048	REAL	ARRAY	Z0
10	R-049	REAL	ARRAY	Z0	27127	RMS	REAL	ARRAY	Z0
14172	P455	REAL	ARRAY	Z0	111	RP	REAL	ARRAY	Z0
164	0P	REAL	ARRAY	Z0	75	SA	REAL	ARRAY	Z0
74	0P	REAL	ARRAY	Z0	77	SC	REAL	ARRAY	Z0
100	0P	REAL	ARRAY	Z0	101	SE	REAL	ARRAY	Z0
102	SG	REAL	ARRAY	Z0	103	SH	REAL	ARRAY	Z0
104	51	REAL	ARRAY	Z0	105	SJ	REAL	ARRAY	Z0
13455	02A	REAL	ARRAY	Z0	15776	SPENT	REAL	ARRAY	Z0
13457	020	REAL	ARRAY	Z0	13454	SUP	REAL	ARRAY	Z0
42	7	REAL	ARRAY	Z0	13516	TACDVT	REAL	ARRAY	Z0
11	TCOI	REAL	ARRAY	Z0	13453	TDMT	REAL	ARRAY	Z0
11	TCOP	REAL	ARRAY	Z0	42	TJ	REAL	ARRAY	Z0
13451	TIME	REAL	ARRAY	Z0	13461	TLPS	REAL	ARRAY	Z0
16272	TR	REAL	ARRAY	Z0	133	TMOX	REAL	ARRAY	Z0
107	TR	REAL	ARRAY	Z0	133	TSEP	REAL	ARRAY	Z0
24647	TTCOI	REAL	ARRAY	Z0	6	TTIME	REAL	ARRAY	Z0
25075	TTMOX	REAL	ARRAY	Z0	16300	TVL	REAL	ARRAY	Z0
16275	TV	REAL	ARRAY	Z0	0	T1A	REAL	ARRAY	Z0
1	T19	REAL	ARRAY	Z0	2	T2	REAL	ARRAY	Z0
3	T1A	REAL	ARRAY	Z0	4	T30	REAL	ARRAY	Z0
5	T4	REAL	ARRAY	Z0	6	T5	REAL	ARRAY	Z0
7	T6	REAL	ARRAY	Z0	16224	VCH	REAL	ARRAY	Z0
13445	VWVS	REAL	ARRAY	Z0	20543	1	REAL	ARRAY	Z0
16303	11	REAL	ARRAY	Z0	16	TVV	REAL	ARRAY	Z0

0 TAPES FMT

4102 PUNCH

2041 OUTPUT
4102 TAPE7

MODE

FILE NAMES
0 INPUT
2041 TAPE6

ARGES

TYPE

EXTERNALS

7	REAL	IMPT
4	REAL	MANCTH
0	REAL	MANCT3
10	REAL	MANCT4
0	REAL	SUP
10	REAL	SUB3

STATEMENT LABELS

11745	1	FMT
12104	4	FMT
12140	2	FMT
12203	5	FMT
10237	3	FMT
0	0	FMT

D

STATEMENT LABELS

13240 10	13237 9	FMT	
13340 11	13345 12	FMT	
13440 12	13382 15	FMT	
13540 13	10101 33		
13640 14	10142 36		
13740 15	0 39		
13840 16	0 51		
13940 17	0 77		
14040 18	0 80		
14140 19	0 171		
14240 20	12417 190	FMT	
14340 21	12441 193	FMT	
14440 22	12501 196	FMT	
14540 23	0 212		
14640 24	12774 246	FMT	
14740 25	12370 301	FMT	
14840 26	12523 300	FMT	
14940 27	13071 402	FMT	
15040 28	0520 499		
15140 29	12561 502	FMT	
15240 30	12614 505	FMT	
15340 31	12647 508	FMT	
15440 32	12702 511	FMT	
15540 33	0 600		
15640 34	6617 621		
15740 35	6735 641		
15840 36	0 640		
15940 37	7101 671		
16040 38	0 680		
16140 39	7215 691		
16240 40	0 710		
16340 41	7403 721		
16440 42	0 740		
16540 43	0 779		
16640 44	12532 3006	FMT NO REFS	

INACTIVE

COMMON BLOCKS LENGTH

13240 10	97
13340 11	80
13440 12	401
13540 13	134
13640 14	45
13740 15	24
13840 16	750
13940 17	272
14040 18	35
14140 19	54
14240 20	10
14340 21	74

STATISTICS

PROGRAM LENGTH	376140	14229
BUFFER LENGTH	61434	7171
COMMON LENGTH	70510	1545
PLANK COMMON	1410	97

11/15/74 13.13.53.

FTN 4.1-PSR367

SUBROUTINE SUB 74/74 OPT=1

```

115      145 IF (FPO.GT.1.1FPO=1.
      17   OT=OAFAR*(1.-FPO)*OP
      17   FRAC=FW*OFF*(NOICH)/OT
      17   IF (FRAC.GT.1.1FRAC=1.
      17   CONTINUE
      17   IF (IPRINT.EQ.1)
      17   WRITE (4,1000)PP,XEQA,EYA,D1.02,D3.04,D5.06,D10
      17   COMPUTE M
      17   A1WR=A11+A12+A13+A14+A15+A16
      17   C=A17+A18
      17   AM9=AT+EQA
      17   AM9A=AT+EQA
      17   AM9B=AT+EQA-A1WR-D1.02-D3.04-D5.06-D7.08
      17   IF (AM9B)20,21,21
      17   YA=AM9B/AM9
      17   YP=8.
      17   GOT022
      17   YP=AM9B/PM9
      17   YA=8.
      17   CONTINUE
      17   AM1=YD*P1*YA*A1
      17   AM2=YD*P2*YA*A2
      17   AM3=YD*P3*YA*A3
      17   AM4=YD*P4*YA*A4
      17   AM5=YD*P5*YA*A5
      17   AM6=YD*P6*YA*A6
      17   AM7=YD*P7*YA*A7
      17   AM8=YD*P8*YA*A8
      17   IF (IPRINT.EQ.1) WRITE (6,1400)A1WR,AM9B
      17   FORMAT (10F8.10)AM9B,7F16.4)
      17   COMPUTE NITRATUM ION CONCENTRATION
      17   F=AO/3A
      17   N=A11/OA
      17   S=A11/OA
      17   IF (A14.GT.0.) GO TO 1341
      17   SUBROUTINE WATER SYSTEM
      17   YL=9.
      17   YU=5.
      17   DO 1304 I=1,40
      17   Y=(YL+YU)/2.
      17   X=IVGY-AMCEN*(S-Y)*(U-Y)/(12.*AMECEN*(S-Y)*Y)
      17   IF (X.LF.0.0001.ELE.(Y-U)/2.) GO TO 1305
      17   GO TO 1306
      17   YL=Y
      17   YU=Y
      17   GO TO 1308
      17   IF IX.GE.F.GR.I.OE.Y) GO TO 1307
      17   GO TO 1308
      17   YU=Y
      17   GO TO 1308
      17   AM1=XOY*U*2.*R-Y)/(F.-21*(S-Y))
      17   IF (AM1-AMECEN).LT.-.001) GO TO 1312
      17   IF (AM1-AMECEN) GO TO 1310
      17   YU=Y
      17   GO TO 1308
      17   YL=Y
      17   GO TO 1308

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345      AS=(A15*05+C10T5)/(4*0F10A+CZ)
      IF (A5.LT.0.) AS=0.
      R10=A5*F10A
      Z4=.0F10P/(4*0F10A+CZ)
      X=A16*016*06-Z*(A16*06)
      Y=Z*CH1.1.
      T6=(16*0TP*01)/(1.0TP*01)
      A6=(A16*06+C10T6)/(4*0F10A+CZ)
      IF (A6.LT.0.) A6=0.
      R10=A6*F10A
      P10=10A*0104
      X=A17*017*010
      Y7=(17*0TP*01)/(1.0TP*01)
      A7=(A17*010+C10T7)/CZ
      IF (A7.LT.0.) A7=0.
      X=A18*018*0.0010
      Y8=(18*0TP*01)/(1.0TP*01)
      A8=(A18*0.0010+C10T8)/CZ
      IF (A8.LT.0.) A8=0.

349      C
      C
      AS04=A11*014
      CS=11.007*14.5 000*0.0010*14.5*006
      000F04CS
      CSP=CS*09
      IF (1000T.EQ.1)
        C00ITE (6.1000)01.02.03.04.05.06.07.08.09.10
        AL=013*014
      IF (1000T.EQ.1)00ITE (6.1405)0.0010*0.0010*0.0010
      1405 FORMAT (14H00,DELTA,6A0.0,14.5)
      IF (1000T.NE.1)C0T01700
        D01= (A11*01-03*01*AM1-A1)
        D02 = (A12*02-04*02*AM2-A2 )
        D03 = (A13*03-05*03*AM3-07A-A3*00A)
        D04 = (A14*04-06*04*AM4-07A-08A-AA*00A)
        D05 = (A15*05-05*05*AM5-R10A-A5)
        D06 = (A16*06-06*06*AM6-R10A-A6)
        D07 = (A17*07-07*07*AM7-A7)
        D08 = (A18*08-08*08*AM8-A8)
      00ITE (6.1450) A10.P10*0.010*0.03.04.05.06.07.08.09.10*0.0010*0.0010*0.0010
      1450 FORMAT (50H010.P10.P0.P10.P3.P4.P5.P6.P7.P8.P9.P10*0.0010*0.0010*0.0010/
      C (12H12.41)
      00ITE (6.1451) A11.A11*0.0.A111.A11*0.0.A114.CSP.A504
      1451 FORMAT (12H0113.A116.A1.A111.A116.CSP.A504/12H12.4)
      D09 = (A19.P19*09-09*09*AM9-13.007-12.5000*0.0010*
      C (1.37*0.67*0010*09-09-12.5000)
      D01 = ( A113-A116*010*03*04*05*06*15.007*16.5000*12.0010-
      C (1.33000*0.67)009*0.16.5000)
      D0504 = (A111.A116-CSP -A504)
      D012 = (A112*012-CSP -A12)
      D01 = (P11-01-AM1-01)
      D02 = (P12-02-AM2-02)
      D03 = (P13-03-AM3-03)
      D04 = (P14-04-AM4-04)
      D05 = (P15 -05-AM5-05)
      D06 = (P16-06-AM6-06)
      D07 = (P17-07-AM7-07)

```

109

SYMBOLIC DIFFERENCE MAP (R=1)

ENTRY POINTS

1 SUB

VARIABLES	SN	TYPE	RELOCATION	ARRAY	REAL	ARRAY	INPUT
0 A	0	REAL	VECTOR		REAL		INPUT
2417 A100	12	REAL			REAL		INPUT
11 A110	13	REAL	INPUT		REAL		INPUT
13 A112	14	REAL	INPUT		REAL		INPUT
15 A114	16	REAL	INPUT		REAL		INPUT
17 A116	20	REAL	INPUT		REAL		INPUT
1 A12	2	REAL	INPUT		REAL		INPUT
3 A14	4	REAL	INPUT		REAL		INPUT
5 A16	6	REAL	INPUT		REAL		INPUT
7 A18	10	REAL	INPUT		REAL		INPUT
1745 AKC	1746	REAL			REAL		
1747 AKC	1750	REAL			REAL		
1751 AKC	2342	REAL			REAL		
2353 AKC	105	REAL			REAL		
77 AKC	73	REAL			REAL		
76 AKC	74	REAL			REAL		
443 AK1	51	REAL			REAL		
44 AK17	47	REAL			REAL		
53 AK75	54	REAL			REAL		
2456 AKC	51	REAL			REAL		
50 AK40	57	REAL			REAL		
57 AK65	2540	REAL			REAL		
40 AKC	2423	REAL			REAL		
2420 AKC	2425	REAL			REAL		
2426 AKC	2427	REAL			REAL		
2430 AKC	2431	REAL			REAL		
2432 AKC	2395	REAL			REAL		
2535 AKC	2397	REAL			REAL		
2345 AK1	0	REAL			REAL		
11 A10	12	REAL			REAL		
2673 A1104	13	REAL			REAL		
16 A17	15	REAL			REAL		
18 A15	17	REAL			REAL		
20 A17	1	REAL			REAL		
2 A1	3	REAL			REAL		
4 A5	5	REAL			REAL		
6 A7	7	REAL			REAL		
10 A9	2454	REAL			REAL		
2451 AK	2455	REAL			REAL		
2452 AK	2455	REAL			REAL		
2450 C	2455	REAL			REAL		
2456 C	2455	REAL			REAL		
2457 C	2455	REAL			REAL		
2458 C	2455	REAL			REAL		
2459 C	2455	REAL			REAL		
2460 C	2455	REAL			REAL		
2461 C	2455	REAL			REAL		
2462 C	2455	REAL			REAL		
2463 C	2455	REAL			REAL		
2464 C	2455	REAL			REAL		
2465 C	2455	REAL			REAL		
2466 C	2455	REAL			REAL		
2467 C	2455	REAL			REAL		
2468 C	2455	REAL			REAL		
2469 C	2455	REAL			REAL		
2470 C	2455	REAL			REAL		
2471 C	2455	REAL			REAL		
2472 C	2455	REAL			REAL		
2473 C	2455	REAL			REAL		
2474 C	2455	REAL			REAL		
2475 C	2455	REAL			REAL		
2476 C	2455	REAL			REAL		
2477 C	2455	REAL			REAL		
2478 C	2455	REAL			REAL		
2479 C	2455	REAL			REAL		
2480 C	2455	REAL			REAL		
2481 C	2455	REAL			REAL		
2482 C	2455	REAL			REAL		
2483 C	2455	REAL			REAL		
2484 C	2455	REAL			REAL		
2485 C	2455	REAL			REAL		
2486 C	2455	REAL			REAL		
2487 C	2455	REAL			REAL		
2488 C	2455	REAL			REAL		
2489 C	2455	REAL			REAL		
2490 C	2455	REAL			REAL		
2491 C	2455	REAL			REAL		
2492 C	2455	REAL			REAL		
2493 C	2455	REAL			REAL		
2494 C	2455	REAL			REAL		
2495 C	2455	REAL			REAL		
2496 C	2455	REAL			REAL		
2497 C	2455	REAL			REAL		
2498 C	2455	REAL			REAL		
2499 C	2455	REAL			REAL		
2500 C	2455	REAL			REAL		
2501 C	2455	REAL			REAL		
2502 C	2455	REAL			REAL		
2503 C	2455	REAL			REAL		
2504 C	2455	REAL			REAL		
2505 C	2455	REAL			REAL		
2506 C	2455	REAL			REAL		
2507 C	2455	REAL			REAL		
2508 C	2455	REAL			REAL		
2509 C	2455	REAL			REAL		
2510 C	2455	REAL			REAL		
2511 C	2455	REAL			REAL		
2512 C	2455	REAL			REAL		
2513 C	2455	REAL			REAL		
2514 C	2455	REAL			REAL		
2515 C	2455	REAL			REAL		
2516 C	2455	REAL			REAL		
2517 C	2455	REAL			REAL		
2518 C	2455	REAL			REAL		
2519 C	2455	REAL			REAL		
2520 C	2455	REAL			REAL		
2521 C	2455	REAL			REAL		
2522 C	2455	REAL			REAL		
2523 C	2455	REAL			REAL		
2524 C	2455	REAL			REAL		
2525 C	2455	REAL			REAL		
2526 C	2455	REAL			REAL		
2527 C	2455	REAL			REAL		
2528 C	2455	REAL			REAL		
2529 C	2455	REAL			REAL		
2530 C	2455	REAL			REAL		
2531 C	2455	REAL			REAL		
2532 C	2455	REAL			REAL		
2533 C	2455	REAL			REAL		
2534 C	2455	REAL			REAL		
2535 C	2455	REAL			REAL		
2536 C	2455	REAL			REAL		
2537 C	2455	REAL			REAL		
2538 C	2455	REAL			REAL		
2539 C	2455	REAL			REAL		
2540 C	2455	REAL			REAL		
2541 C	2455	REAL			REAL		
2542 C	2455	REAL			REAL		
2543 C	2455	REAL			REAL		
2544 C	2455	REAL			REAL		

PTM 4.10-20207 11/15/76 13.13-53.

76/76 OPT=1

FILE NAMES MODE
TAPES PWT

INLAP FUNCTIONS TYPE ADDS
MS REAL 1 BINARY

STATEMENT LABELS

1763 1	PWT	1720 3	INACTIVE
0 4		0 11	INACTIVE
127 17		0 15	INACTIVE
253 34		0 20	INACTIVE
350 21		0 30	INACTIVE
1687 71		0 141	INACTIVE
0 147		0 144	INACTIVE
302 105		2915 1000	PWT
444 1700		442 1306	
445 1397		443 1310	
647 1112		2306 140-	PWT
2276 1401	PWT	2123 1405	PWT
2041 1400	PWT	2173 1451	PWT
2220 1740	PWT	1520 1700	
522 2117		550 2339	
352 2740		0 2342	INACTIVE
355 2743		573 2345	
577 2746		443 2351	
614 1700			

COMMON BLOCKS LENGTH
BOYS 10
// 97
VECTOR 45
END 04
INOUT 35
END 24
70

STATISTICS
PROGRAM LENGTH 25740 1443
COMMON LENGTH 4700 740
BLANK COMMON 1410 97

FTW 4.1-PSR367 11/15/74 13.14.10.

SUBROUTINE SUB2 74/74 OPT=1

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS

3 4192

VARIABLES	SN	TYPE	RELUCATION
3 AKNA	REAL		Z0
61 AK10	REAL		Z0
53 AK15	REAL		Z0
54 AK16	REAL		Z0
51 AK15	REAL		Z0
57 AK7	REAL		Z0
0 40	REAL		F.P.
16 CP	REAL		Z0
0 FAMP	REAL		F.P.
71 F19	REAL		Z0
55 F15	REAL		Z0
54 F15	REAL		Z0
65 F55	REAL		Z0
67 F7	REAL		Z0
0 F49	REAL		F.P.
72 F0	REAL		Z0
110 F01	REAL		Z0
0 F01	REAL		F.P.
153 1	INTEGER		
0 P0	REAL		F.P.
151 P4	REAL		
154 P1	REAL		
111 P0	REAL		Z0
75 S4	REAL		Z0
77 SC	REAL		Z0
101 CE	REAL		Z0
103 CH	REAL		Z0
105 CJ	REAL		Z0

FILE NAMES MODE
TAMEG FMT

STATEMENT LABELS

124 1 FMT

0 28

0 58 INACTIVE

COMMON BLOCKS LENGTH
70 74

STATISTICS

PROGRAM LENGTH 1628 114
COMMON LENGTH 1128 74

74 ANMATH	REAL		
46 AK12	REAL		Z0
47 AK30	REAL		Z0
50 AK40	REAL		Z0
42 AK65	REAL		Z0
48 AK0	REAL		Z0
147 AT	REAL		Z0
34 OH	REAL		F.P.
0 EOMP	REAL		Z0
42 E21	REAL		Z0
63 E30	REAL		Z0
44 E40	REAL		Z0
44 E65	REAL		Z0
70 E8	REAL		F.P.
0 F401	REAL		F.P.
155 F7	REAL		F.P.
0 F70	REAL		F.P.
0 FRAC	REAL		F.P.
0 NOTCH	REAL		F.P.
150 PT	REAL		
142 CP	REAL		Z0
0 P40	REAL		Z0
100 P0	REAL		Z0
76 S0	REAL		Z0
100 S0	REAL		Z0
102 S6	REAL		Z0
144 S1	REAL		Z0
147 TH	REAL		Z0

0 10
50 40

FMT INACTIVE

141 2
0 30
62 60

[illegible]

FTW 4.1-PSB367 11/15/74 13.14.14.

SUBROUTINE SUBI 74/74 OPT=1

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS

3 SUBI

VARIABLES	SM	TYPE	RELOCATION	F.P.
0 AT	REAL			
74 AKWATL	REAL	ARRAY	ZO	
66 AK12	REAL		ZO	
47 AK3M	REAL		ZO	
50 AK4M	REAL		ZO	
52 AK6S	REAL		ZO	
69 AKR	REAL		ZO	
0 AV	REAL		ZO	
737 CHAMXO	REAL	ARRAY	VECT	
134 MFA	REAL		VECT	
734 CHAMXO	REAL	ARRAY	VECT	
133 MFMX	REAL		VECT	
34 FM	REAL	ARRAY	ZO	
0 FX	REAL		//	
62 F21	REAL		ZO	
63 F3M	REAL		ZO	
64 F4M	REAL		ZO	
66 F6S	REAL		ZO	
70 F8	REAL		ZO	
110 FMX	REAL		ZO	
110 G18	REAL	ARRAY	PAR	
30 G3S	REAL	ARRAY	PAR	
40 G4S	REAL	ARRAY	PAR	
60 G6	REAL	ARRAY	PAR	
100 G8	REAL	ARRAY	PAR	
132 I	INTEGER		//	
2 IPONT	INTEGER		//	
3 JACK	INTEGER		//	
5 NM	INTEGER		//	
356 OV	REAL	ARRAY	VECT	
13 OATES	REAL		//	
11 O-O10	REAL		ZO	
13 OHO12	REAL		ZO	
15 OHO14	REAL		ZO	
2 OHO17	REAL		ZO	
4 OHO5	REAL		ZO	
6 OHO7	REAL		ZO	
10 OHO9	REAL		ZO	
104 O9	REAL		ZO	
11 O10	REAL		ZO	
2 O3	REAL		DUM	
4 O5	REAL		DUM	
6 O7	REAL		DUM	
10 O9	REAL		DUM	
76 O8	REAL		ZO	
100 O9	REAL		ZO	
102 O6	REAL		ZO	
104 O1	REAL		ZO	
11 TCOR	REAL		//	
107 TB	REAL		ZO	
73 ANWA	REAL		ZO	
61 AN10	REAL		ZO	
53 AK3S	REAL		ZO	
54 AK4S	REAL		ZO	
51 AK5S	REAL		ZO	
57 AK7	REAL		ZO	
0 AD	REAL		ZO	
735 CHAM10	REAL	ARRAY	VECT	
16 CP	REAL	ARRAY	VECT	
131 OFARX	REAL		ZO	
152 OFP	REAL	ARRAY	VECT	
740 OFPMD	REAL		VECT	
1 DT	REAL		//	
71 E10	REAL		ZO	
55 E3S	REAL		ZO	
56 E4S	REAL		ZO	
55 E5S	REAL		ZO	
07 E7	REAL		ZO	
12 F0	REAL		ZO	
0 G1	REAL	ARRAY	PAR	
10 G3	REAL	ARRAY	PAR	
20 G4	REAL	ARRAY	PAR	
50 G5	REAL	ARRAY	PAR	
70 G7	REAL	ARRAY	PAR	
120 G9	REAL	ARRAY	PAR	
7 TCALL	INTEGER		//	
734 IVSL	INTEGER		VECT	
4 NM	INTEGER		//	
10 NP	INTEGER		//	
0 OY	REAL	ARRAY	F.P.	
0 RH01	REAL		ZO	
12 RH011	REAL		ZO	
14 RH013	REAL		ZO	
1 RH02	REAL		ZO	
3 RH04	REAL		ZO	
5 RH06	REAL		ZO	
7 RH08	REAL		ZO	
111 RP	REAL		ZO	
0 R1	REAL		DUM	
1 R2	REAL		DUM	
3 R4	REAL		DUM	
5 R6	REAL		DUM	
7 R8	REAL		DUM	
75 SA	REAL		ZO	
77 SC	REAL		ZO	
101 SE	REAL		ZO	
103 SH	REAL		ZO	
105 SJ	REAL		ZO	
12 TROX	REAL		//	
133 TSEP	REAL	ARRAY	//	

FTN 4.1-PSH357 11/15/74 13.14.14.

11/74 OPT=1

RELOCATION
//

16 XTY REAL ARRAY 000

FILE NAMES
TAPE6 PNT

INLINE FUNCTIONS TYPE ARGS
ANS DEAL 3 INTRIN

STATEMENT LABELS

0 90 INACTIVE
0 114
0 113
17 125
63 134

0 96
0 111
0 123
20 126
0 135

INACTIVE
INACTIVE
INACTIVE

101 87 PNT
122 112 PNT
0 124
0 133
45 136

INACTIVE
INACTIVE

COMMON BLOCKS LENGTH
// 97
000 29
VECT 408
FUM 18
PAR 84
70 74

STATISTICS

PROGRAM LENGTH 1708 120
COMMON LENGTH 12518 681
PLANK COMMON 1418 97

[illegible]

FTN 4.1-PSB367 11/15/74 13.14.17.

74/74 OPT=1

CIRCUITRY INPT

STATEMENT LABELS

51 20
41 48
0 71
245 160
545 112
557 744
155 774

33 21
45 45
0 72
464 110
152 171
417 349
0 779

25 38
0 70
217 91
506 111
611 383
52 777

PMT
PMT

PMT

PMT

INACTIVE

COMMON BLOCKS LENGTH

040 46
70 74
PMT 54
CST 146
T 138
/ / 97

STATISTICS

PROGRAM LENGTH 14038
COMMON LENGTH 10128
PLANE COMMON 1418

771
522
97

125

SYMBOLIC REFERENCE MAP (R011)

(KIRY PRINTS
2 FTN)

VARIABLES	SN	TYPE	RELOCATION
157 A		REAL	
74 ARWAL		REAL	20
44 AR12		REAL	20
47 AR14		REAL	20
50 AR16		REAL	20
52 AR18		REAL	20
48 AR10		REAL	20
14 CP		REAL	20
31 CP12		REAL	20
33 CP14		REAL	20
34 CM		REAL	20
143 FRTM		REAL	
154 FRTM2		REAL	
62 F21		REAL	20
63 F24		REAL	20
64 F26		REAL	20
66 F28		REAL	20
70 F4		REAL	20
72 F3		REAL	20
146 T		INTEGER	
144 LPS		REAL	
174 P		REAL	
0 P-01		REAL	20
12 P-011		REAL	20
14 P-013		REAL	20
1 P-02		REAL	20
3 P-04		REAL	20
5 P-06		REAL	20
7 P-08		REAL	20
106 P		REAL	20
74 CR		REAL	20
100 CD		REAL	20
102 CG		REAL	20
104 CI		REAL	20
154 T		REAL	20
107 TR		REAL	20
155 UTM		REAL	20
0 VAL		REAL	20
0 V01		REAL	20
231 Y		REAL	
73 ANNA		REAL	
61 AN10		REAL	
53 AN35		REAL	
54 AN45		REAL	
51 AN55		REAL	
57 AN7		REAL	
0 AI		REAL	
30 CP11		REAL	
32 CP13		REAL	
26 CP9		REAL	
147 BLV		REAL	
153 EXTH0		REAL	
71 E10		REAL	
95 E35		REAL	
56 E45		REAL	
65 E55		REAL	
67 E7		REAL	
151 F		REAL	
110 FMAX		REAL	
152 J		INTEGER	
145 LPS		REAL	
0 P1		REAL	
11 P-010		REAL	
13 P-012		REAL	
15 P-014		REAL	
2 P-03		REAL	
4 P-05		REAL	
6 P-07		REAL	
10 P-09		REAL	
75 SA		REAL	
77 SC		REAL	
101 SE		REAL	
103 SN		REAL	
105 SJ		REAL	
0 TP		REAL	
159 UTA		REAL	
213 I		REAL	
0 K42		REAL	
0 W2		REAL	

INLINE FUNCTIONS TYPE
FLOAT
1 INTRIN

STATEMENT LABELS

129 1
0 10

COMMON BLOCKS LENGTH
73

187 2

186 3

3

PAGE

11/15/76 13:14:22

FTN 4.1092267

76/76 07102

FUNCTION ENVR

STATISTICS

PROGRAM LENGTH

2458

101

73

118

CORE MAP	18.04.84. NORMAL	CONTROL	USER	CALL	000100	067525	067364	000141
TIME	LOAD MODE	TYPE	COMMON	ADDRESS	FMA LOAD	LWA LOAD	BLNK COMM	LENGTH
FMA LOAD	123645	FMA TABLES	114403					
PROGRAM	ADDRESS							
NANC30	000570							
NANC30	001613							
NANCYM	003733							
RTHETA	005074							
NANCYL	005110							
NANPLY	005221							
NANC3V	005554							
NANX	005673							
NUCHAR	005770							
LABEL	006076							
TITLE	006143							
LYNHN	006226							
SA/PLI	006234							
TNTSIM	011341							
SUB	053277							
SUB2	056255							
SUB1	056520							
INPT	056773							
ENTH	060421							
GETRA	060711							
SIO8	060730							
SYSTEMS	062371							
ACGNERS	063401							
IMPUTCS	063414							
KODERS	063543							
KRAKERS	065156							
OUTPTCS	066710							
ARSS	067004							
INTS	067007							
FLOATS	067012							
ALMLOGE	067015							
ERPS	067054							
EXPE	067116							
LEGVARS	067162							

REMARKS 067157
SINCOSE 067217
XTCIE 067274
XTQYS 067311
-----UNSATISFIED EXTERNALS-----

REFERENCES

INPUT COMPS

2369	.0098	.0596	.0021	.0267	.0014	.0000	.0000	17.7404	0.0000
98.4475	7.2890	166.7045	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	5.1237	.0002
19.5969	.0134	4.7095	.1650	2.1800	.1650	.0000	.0000	18.3440	0.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	5.2285	.0011
.1626	.0007	.0348	.0012	.0162	.0000	-0.0000	-0.0000	18.3436	0.0000
115.7939	0.5315	225.2497	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	5.2284	.0011
22.2942	.9181	4.7744	.1684	2.2202	.1135	.0000	.0000	32.0027	0.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	7.4833	.0000
.1622	.0066	.0352	.0013	.0162	.0000	-0.0000	-0.0000	31.9137	0.0000
115.7934	4.5315	225.2502	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	7.4702	.0000
22.2942	.5181	4.7744	.1684	2.2202	.1135	.0000	.0000	28.6507	0.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	.0000
.0155	.0012	.0947	.0316	.5307	.0000	-0.0000	-0.0000	0.0000	.0000
150.1290	11.0750	121.2359	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	.0000
1.1246	.0701	31.1216	1.0958	18.6797	.9397	.0000	.0000	0.0000	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	.0000
.0000	.0000	.0542	.0264	.5718	.0000	-0.0000	-0.0000	0.0000	.0000
150.0900	11.1179	121.3574	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	.0000
1.1946	.0701	31.1240	1.0959	18.6813	.9398	.0000	.0000	0.0000	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	.0000
.0000	.0000	.0542	.0264	.5718	.0000	-0.0000	-0.0000	0.0000	.0000
170.5098	13.0381	14.8901	14.4378	3.0878	.1621	.0000	.0000	0.0000	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	.0000
.0000	.0000	.0542	.0264	.5718	.0000	-0.0000	-0.0000	0.0000	.0000
177.5596	13.4703	1.7454	.0168	10.1950	.4710	.0000	.0000	0.0000	.0000
.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	.0000
.0000	.0000	.0542	.0264	.5718	.0000	-0.0000	-0.0000	0.0000	.0000
167.1102	7.2422	3.1125	.0336	40.8936	1.7818	.0000	.0000	0.0000	.0000
.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	.0000
.0000	.0000	.0542	.0264	.5718	.0000	-0.0000	-0.0000	0.0000	.0000
167.5583	7.4483	3.1143	.0336	40.1764	1.7854	.0000	.0000	0.0000	.0000
.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	.0000
.0000	.0000	.0542	.0264	.5718	.0000	-0.0000	-0.0000	0.0000	.0000
94.1930	1.4421	0.0000	.0018	11.6526	.4999	.0000	.0000	0.0000	.0000
.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	.0000
.0000	.0000	.0542	.0264	.5718	.0000	-0.0000	-0.0000	0.0000	.0000
94.3154	1.4498	0.0000	.0018	11.6526	.4999	.0000	.0000	0.0000	.0000
.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	.0000
.0000	.0000	.0542	.0264	.5718	.0000	-0.0000	-0.0000	0.0000	.0000
72.3983	.2300	0.0000	.0018	11.6526	.4999	.0000	.0000	0.0000	.0000
.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	.0000
.0000	.0000	.0542	.0264	.5718	.0000	-0.0000	-0.0000	0.0000	.0000
72.4159	.2448	0.0000	.0018	11.6526	.4999	.0000	.0000	0.0000	.0000
.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	.0000
.0000	.0000	.0542	.0264	.5718	.0000	-0.0000	-0.0000	0.0000	.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	.0000
.0000	.0000	.0542	.0264	.5718	.0000	-0.0000	-0.0000	0.0000	.0000

*****INPUT DATA*****

PATE CONSTANTS

K12 K31 K41 K51 K61 K71 K81 K91
24.802503330.00 322403.00 671000.00 571000.00 506.76 1.33 1.33 1.33

ACTIVATION ENERGIES

E21 E31 E41 E51 E61 E71 E81 E91
09. 24000. 17442. 17200. 10400. 6500. 6300. 10000. 1.

CONSTANTS

A B C D E F G H I J
44 5000.00 4.27 1.55 2.00 7000.00 4.9560000.00 .36

GAS LAW CONSTANT = .90

REFERENCE TEMPERATURE = 343.30 DEG K

MASS TA. COEFF. = 20000.0

MASS TA. COEFF. (TOL) = 5000.0

CONVERSION OF MAOS04 DECOMPOSITION REACTION = .5618

OXYGEN COEFFICIENT = .7000

PHYSICAL PROPERTIES

COMPONENT	MOL. WT.	DENSITY	WT. CAP.	REACTION	MT. OF REACTION
1	137.0	.50	33.40	1	15340.
2	137.0	.50	33.80	2	15010.
3	182.0	.46	33.80	3	15000.
4	182.0	.46	33.80	4	14920.
5	227.0	.40	33.80	5	11260.
6	227.0	.40	33.80	6	14520.
7	213.0	.40	33.80	7	237000.
8	258.0	.40	33.80	8	321000.
9	61.0	1.45	16.01	9	16300.
10	42.0	.55	33.09	10	0.
11	94.0	1.15	15.55		
12	176.0	1.15	0.00		
13	18.0	3.39	8.16		
14	60.0	1.15	14.30		

STAGE 1
NITRATOR 1A
VOL. = 52.1
TEMP. = 24.0

SEPARATOR 1
VOL. = 20.1
NOTCH SETTING = 1
ENTRAINMENT
ORGANIC IN ACID .00071
ACID IN ORGANIC 9.00000

STAGE 2
NITRATOR 2
VOL. = 48.1
TEMP. = 40.0

SEPARATOR 2
VOL. = 20.1
NOTCH SETTING = 2
ENTRAINMENT
ORGANIC IN ACID .02787
ACID IN ORGANIC .15615

STAGE 3
NITRATOR 3A
VOL. = 53.5
TEMP. = 76.0

SEPARATOR 3
VOL. = 20.1
NOTCH SETTING = 3
ENTRAINMENT
ORGANIC IN ACID .09532
ACID IN ORGANIC .13910

STAGE 4
NITRATOR 4
VOL. = 53.5
TEMP. = 92.0

SEPARATOR 4
VOL. = 20.1
NOTCH SETTING = 4
ENTRAINMENT
ORGANIC IN ACID .03067
ACID IN ORGANIC .02421

STAGE 5
NITRATOR 5
VOL. = 60.2
TEMP. = 100.0

SEPARATOR 5
VOL. = 20.1
NOTCH SETTING = 2
ENTRAINMENT
ORGANIC IN ACID .04133
ACID IN ORGANIC .01950

STAGE 6
NITRATOR 6

VOL. = 60.2
TEMP. = 195.8

SEPARATION 8

VOL. = 20.1

NOTCH FITTING = 1

ENTRAINMENT

ORGANIC IN ACID .04715
ACID IN ORGANIC .00477

SUB2	1	.1451	.0000	1.0000	.9927	0.0000	.0073
PT.AT.OP.OA.FWL.FF.OI	35.7183	369.1415	64.3379	180.0040	410.0000	.0453	100.5698
SUB2	2	.3230	.0287	.1950	.9607	.0303	.1450
PT.AT.OP.OA.FWL.FF.OI	66.5750	315.9651	126.7222	201.0040	410.0000	.1655	214.1455
SUB2	3	.4301	.1054	.1516	.9703	.0217	.4343
PT.AT.OP.OA.FWL.FF.OI	58.6837	265.0490	140.2071	227.6231	410.0000	.2918	203.5696
SUB2	4	.5622	.0314	.0240	.9974	.0026	.2203
PT.AT.OP.OA.FWL.FF.OI	45.1100	328.6110	110.7546	294.7274	410.0000	.4294	319.2423
SUB2	2	.3294	.0431	.0199	.9906	.0034	.2011
PT.AT.OP.OA.FWL.FF.OI	44.6257	290.0197	110.2655	140.4270	410.0000	.1655	209.9542
SUB2	1	.1595	.0495	.0440	.9993	.0007	.2640
PT.AT.OP.OA.FWL.FF.OI	31.2105	167.9169	77.2500	151.1100	410.0000	.0453	171.5666

[illegible]

[illegible]

SEPARATION 6

[illegible][illegible][illegible]

5. Answers

[illegible][illegible][illegible]

55-20247-6

[illegible]

[illegible][illegible][illegible][illegible]

[illegible]

INTERNAL ACID RECYCLE		169.695		.439		170.134	
ACID PH.	ADMT	WDMT	ADMT	WDMT	TMS	TURA	M403
.027	.081	.000	.003	.000	.000	.000	2.372
.023	.081	.000	.003	.000	.000	.000	.695
OPG. PH.	ACID PH.	OPG. PH.	OPG. PH.	TOTAL			
	52.325		.837	52.362			
MOLES	WASS		2592.713	2594.804			
VOLUME			27.296	.071			
				27.366			

SEPARATE ?

[illegible]

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DIFFERENTIAL ACID RECYCLE

[illegible]

SEPTEMBER 3

SEPARATION 3									
O-GASIC STREAM TO NEXT STAGE									
	ACID P4	ACID P5	ACID P6	MOIST	ATM	WATER	TOTAL	WATER	TOTAL
ACID P4	.000	.000	.000	.001	.266	.000	.000	.000	.000
ACID P5	.000	.000	.000	.000	23.710	.000	.000	.000	.000
ACID P6	.000	.000	.000	.000	1.224	.000	.000	.000	.000
MOIST	.000	.000	.000	.000	.000	.000	.000	.000	.000
ATM	.000	.000	.000	.000	.000	.000	.000	.000	.000
WATER	.000	.000	.000	.000	.000	.000	.000	.000	.000
TOTAL	.000	.000	.000	.000	.000	.000	.000	.000	.000
MOLES	5.666	5.666	5.666	35.869	40.735	.000	.000	.000	.000
WATER	575.727	575.727	575.727	7504.602	8080.330	.000	.000	.000	.000
WATER	5.343	5.343	5.343	83.895	89.230	.000	.000	.000	.000
TOTAL	586.436	586.436	586.436	8394.366	8969.565	.000	.000	.000	.000
WATER	5.343	5.343	5.343	83.895	89.230	.000	.000	.000	.000
TOTAL	586.436	586.436	586.436	8394.366	8969.565	.000	.000	.000	.000
WATER	5.343	5.343	5.343	83.895	89.230	.000	.000	.000	.000
TOTAL	586.436	586.436	586.436	8394.366	8969.565	.000	.000	.000	.000
WATER	5.343	5.343	5.343	83.895	89.230	.000	.000	.000	.000
TOTAL	586.436	586.436	586.436	8394.366	8969.565	.000	.000	.000	.000
WATER	5.343	5.343	5.343	83.895	89.230	.000	.000	.000	.000
TOTAL	586.436	586.436	586.436	8394.366	8969.565	.000	.000	.000	.000
WATER	5.343	5.343	5.343	83.895	89.230	.000	.000	.000	.000
TOTAL	586.436	586.436	586.436	8394.366	8969.565	.000	.000	.000	.000
WATER	5.343	5.343	5.343	83.895	89.230	.000	.000	.000	.000
TOTAL	586.436	586.436	586.436	8394.366	8969.565	.000	.000	.000	.000
WATER	5.343	5.343	5.343	83.895	89.230	.000	.000	.000	.000
TOTAL	586.436	586.436	586.436	8394.366	8969.565	.000	.000	.000	.000
WATER	5.343	5.343	5.343	83.895	89.230	.000	.000	.000	.000
TOTAL	586.436	586.436	586.436	8394.366	8969.565	.000	.000	.000	.000
WATER	5.343	5.343	5.343	83.895	89.230	.000	.000	.000	.000
TOTAL	586.436	586.436	586.436	8394.366	8969.565	.000	.000	.000	.000
WATER	5.343	5.343	5.343	83.895	89.230	.000	.000	.000	.000
TOTAL	586.436	586.436	586.436	8394.366	8969.565	.000	.000	.000	.000
WATER	5.343	5.343	5.343	83.895	89.230	.000	.000	.000	.000
TOTAL	586.436	586.436	586.436	8394.366	8969.565	.000	.000	.000	.000
WATER	5.343	5.343	5.343	83.895	89.230	.000	.000	.000	.000
TOTAL	586.436	586.436	586.436	8394.366	8969.565	.000	.000	.000	.000
WATER	5.343	5.343	5.343	83.895	89.230	.000	.000	.000	.000

FTYEBW ACID RECYCLE

EXTERNAL ACID RECYCLE											
	AMT	AMNT	MDNT	ATMT	MTNT	TMB4	MM03	TOL	M2S04	M20	S03
ACT(1) P.M.	.000	.014	.599	4.991	.342	.000	18.384	0.000	167.885	8.308	7.427
ACT(2) P.M.	.039	.000	4.855	10.611	.548	.000	0.000	.000			
					TOTAL						
		ACID PM	ORG. PM								
MGLES		144.955	15.695		164.640						
MASS		15134.882	3350.561		18491.442						
MOLEF		148.468	37.546		178.006						

INTERPOL ACIS RECYCLE

[illegible]

SEPARATOR &
ORGANIC STREAM TO NEXT STAGE

[illegible][illegible][illegible]

SEPARATED 5
ORGANIC STREAM TO NEXT STAGE

[illegible][illegible][illegible]

STAFF TO THE CHIEF OF POLICE

[illegible]

EXTERNAL ACID RECYCLE														
	AMNT	MMNT	ADMT	MDMT	ATMT	MTMT	TMT	TMTA	MMO3	TOL	H2SO4	MMO504	H2O	503
ACID PH.	.000	.000	.003	.000	4.820	.285	.000	.000	28.082	0.000	69.289	.329	0.000	47.387
ORG. PH.	.000	.000	.032	.000	7.224	.307	.000	.000	0.000	0.000				
ACID PH.						TOTAL								
MOLES		152.839		7.563		160.402								
MASS		14042.362		1715.364		15757.726								
VOLUME		133.426		18.711		156.137								

INTERNAL ACID RECYCLE														
	AMNT	MMNT	ADMT	MDMT	ATMT	MTMT	TMT	TMTA	MMO3	TOL	H2SO4	MMO504	H2O	503
ACID PH.	.000	.000	.001	.000	1.189	.050	.000	.000	4.998	0.000	11.977	.057	0.000	8.187
ORG. PH.	.000	.000	.005	.000	1.250	.053	.000	.000	0.000	0.000				
ACID PH.						TOTAL								
MOLES		24.458		1.389		27.738								
MASS		2430.102		296.052		2726.955								
VOLUME		24.128		3.238		27.366								

34170	5053.9	22024	21.153	22.104	8.9006	2.0745	16120.37
34134	5054.2	22049	21.163	22.150	8.8951	2.0732	16120.82
34101	5054.9	22071	21.174	22.207	8.8897	2.0719	16121.72
34071	5055.4	22092	21.186	22.242	8.8845	2.0707	16121.48
34044	5057.3	22010	21.190	22.294	8.8797	2.0694	16121.27
34020	5059.0	22024	21.213	22.331	8.8753	2.0680	16121.10
34000	5061.0	22044	21.224	22.365	8.8715	2.0677	16120.97
33941	5061.3	22055	21.264	22.394	8.8682	2.0669	16120.86
33906	5065.0	22071	21.260	22.420	8.8655	2.0663	16120.79
33852	5064.6	22083	21.276	22.441	8.8634	2.0658	16120.76
33841	5071.6	22094	21.293	22.450	8.8619	2.0655	16120.75
33832	5074.7	22003	21.311	22.473	8.8611	2.0653	16120.70
33826	5077.9	22017	21.324	22.483	8.8608	2.0652	16120.62
33810	5081.3	22020	21.346	22.490	8.8610	2.0652	16120.68
33813	5084.7	22027	21.363	22.495	8.8617	2.0654	16120.95
33810	5086.1	22033	21.385	22.497	8.8629	2.0657	16121.01
33807	5091.6	22039	21.397	22.496	8.8644	2.0660	16121.05
33805	5095.1	22044	21.413	22.496	8.8663	2.0665	16121.06
33803	5099.5	22049	21.420	22.498	8.8684	2.0679	16121.04
33801	5101.9	22054	21.444	22.485	8.8708	2.0675	16120.90
33800	5105.3	22059	21.450	22.486	8.8734	2.0681	16120.97
33804	5108.5	22063	21.471	22.474	8.8767	2.0694	16120.71
33805	5111.7	22068	21.484	22.468	8.8799	2.0694	16120.50
33803	5114.8	22073	21.494	22.462	8.8819	2.0701	16120.25
33800	5117.7	22077	21.509	22.457	8.8849	2.0708	16120.95
33806	5120.5	22082	21.520	22.452	8.8880	2.0715	16120.61
33811	5123.2	22088	21.530	22.448	8.8910	2.0722	16120.24
33815	5125.7	22093	21.533	22.445	8.8941	2.0730	16120.84
33809	5128.1	22099	21.544	22.443	8.8971	2.0737	16120.41
33811	5130.4	22104	21.554	22.441	8.9002	2.0744	16121.96
33813	5132.5	22110	21.563	22.441	8.9032	2.0751	16123.49
33815	5134.5	22117	21.579	22.442	8.9061	2.0758	16123.81
33813	5136.4	22123	21.576	22.443	8.9090	2.0764	16122.53
33822	5139.1	22129	21.597	22.446	8.9118	2.0771	16122.05
33815	5141.8	22134	21.597	22.450	8.9146	2.0778	16121.56
33817	5141.3	22142	21.592	22.454	8.9173	2.0784	16121.09
33814	5142.7	22149	21.597	22.459	8.9199	2.0790	16120.61
33819	5144.0	22154	21.601	22.465	8.9225	2.0794	16120.15
33816	5145.2	22162	21.605	22.472	8.9250	2.0802	16119.70
33817	5146.4	22168	21.608	22.479	8.9274	2.0807	16119.25
33820	5147.5	22175	21.617	22.487	8.9297	2.0813	16118.03

1803093.7	600695.2	2164410.3	1130399.8	870792.6	1119507.1	61975.4	125236.4
1803169.5	605580.7	2162636.3	1129759.4	876427.3	1120182.2	620400.4	125751.2
1803172.8	606478.0	2160830.7	1127193.0	870050.9	1120974.5	621229.1	126158.0
1803183.0	600390.2	2159013.0	1126764.6	869712.7	1122502.5	621933.0	126467.0
1802959.9	600317.8	2157203.1	1125757.3	869399.7	1124453.0	622580.3	126722.2
1802765.3	600268.0	2155211.1	1125130.5	869135.6	1125175.2	623109.2	126932.2
1802621.6	600216.4	2153092.3	1124070.3	868727.7	1125403.2	623737.0	127100.2
1802121.9	602186.4	2152033.9	1124491.8	868480.1	1126111.7	624236.3	127250.4
1801721.5	600171.5	2150465.4	1124442.9	86822.4	1126445.8	624693.0	127390.0
1801247.1	605171.5	2149044.4	1123791.1	865659.8	1127514.3	625113.4	127504.4
1801235.9	605187.5	2147736.0	1123132.1	86577.7	1127145.2	625504.4	127600.5
1800957.6	600221.5	2146567.9	1122615.4	864739.4	1128004.2	625470.7	127704.0
1800772.0	600271.0	2145531.1	1122021.6	864437.0	1128623.9	626217.0	127793.0
1800345.5	600332.3	2144648.8	1121464.4	864004.0	1130305.1	626546.7	127877.1
1800241.0	600423.0	2143444.0	1121170.0	863113.4	1131163.3	626967.3	127957.2
1800264.6	600530.9	2143269.3	1121378.5	862980.1	1131913.2	627105.5	128033.7
1800134.9	600647.0	2142776.4	1121376.0	862559.3	1132644.1	627457.4	128107.0
1800131.1	600776.6	2142386.0	1121332.7	862444.2	1133454.8	627736.5	128176.9
1800111.2	6007911.2	2142100.1	1121354.1	862437.5	1134213.2	628009.2	128243.1
1800762.8	601054.0	2141403.4	1121354.5	862260.0	1134975.0	628268.4	128305.4
1800721.5	601290.3	2141142.4	1121353.6	862226.0	1135721.1	628519.2	128363.5
1800363.0	601340.3	2141125.5	1121347.6	86219.3	1136454.5	628750.5	128417.2
1800119.9	601444.9	2141120.4	11213457.3	86218.6	1137174.2	628987.1	128466.1
1800114.7	601639.5	21411756.4	11213430.3	870610.6	1137470.0	629205.1	128510.3
1800171.4	601774.5	2141123.4	1121345.4	870495.1	1138554.1	629412.5	128549.6
1800114.8	601910.5	2141112.4	1121346.0	871109.1	1139246.7	629603.2	128584.2
1800134.1	602040.7	2141015.9	1121346.7	871344.2	1139947.3	629795.4	128614.0
1800174.4	602145.3	2142126.7	1121349.7	871455.3	1140535.7	629971.2	128633.4
1800170.7	602276.0	2142238.4	1121351.3	871639.9	1141155.5	630136.6	128660.5
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MITICIDAL/ACARIC RATIO IN EACH NITRATOR

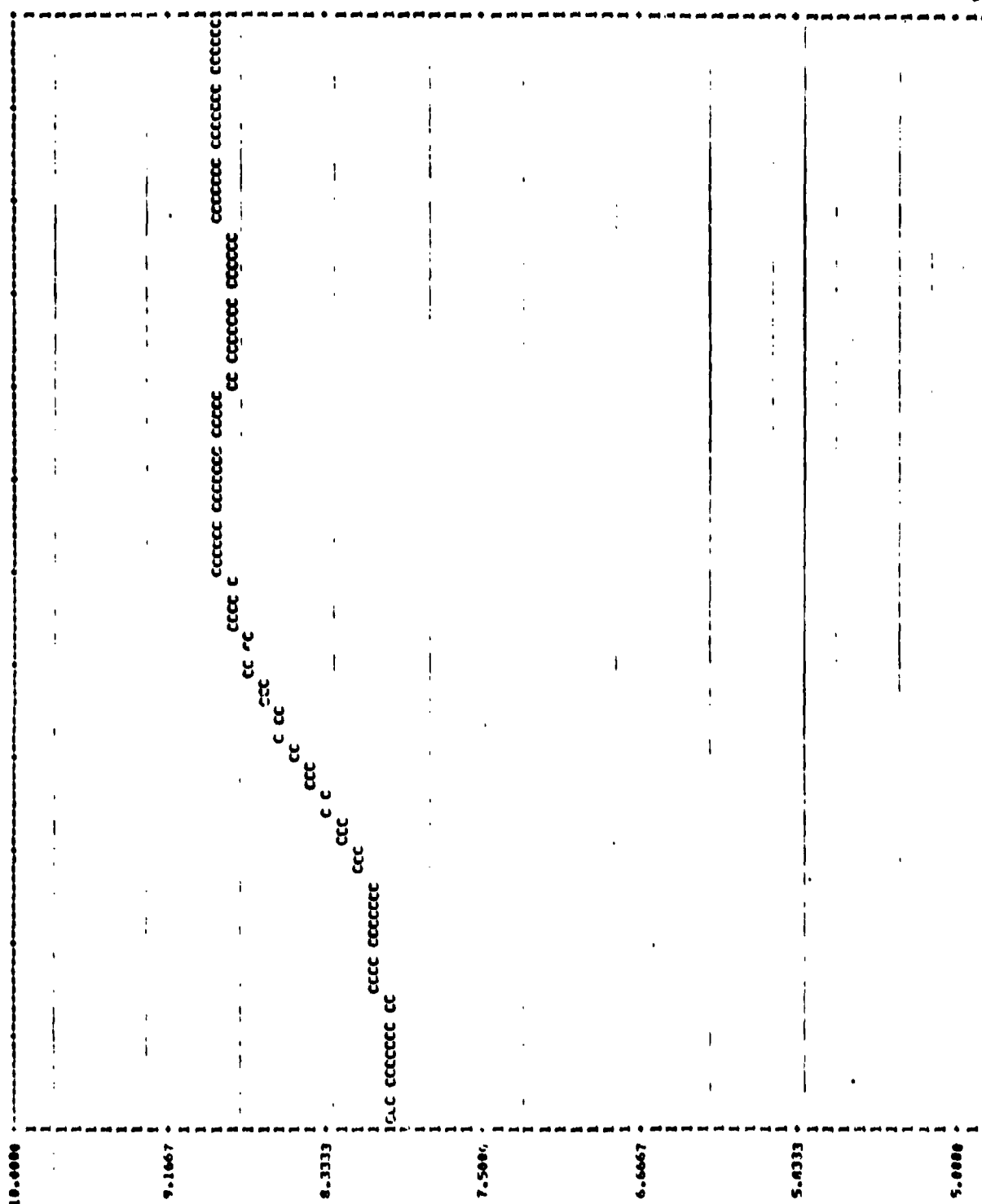
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TIME BETWEEN POINTS = 5.16240 MINUTES



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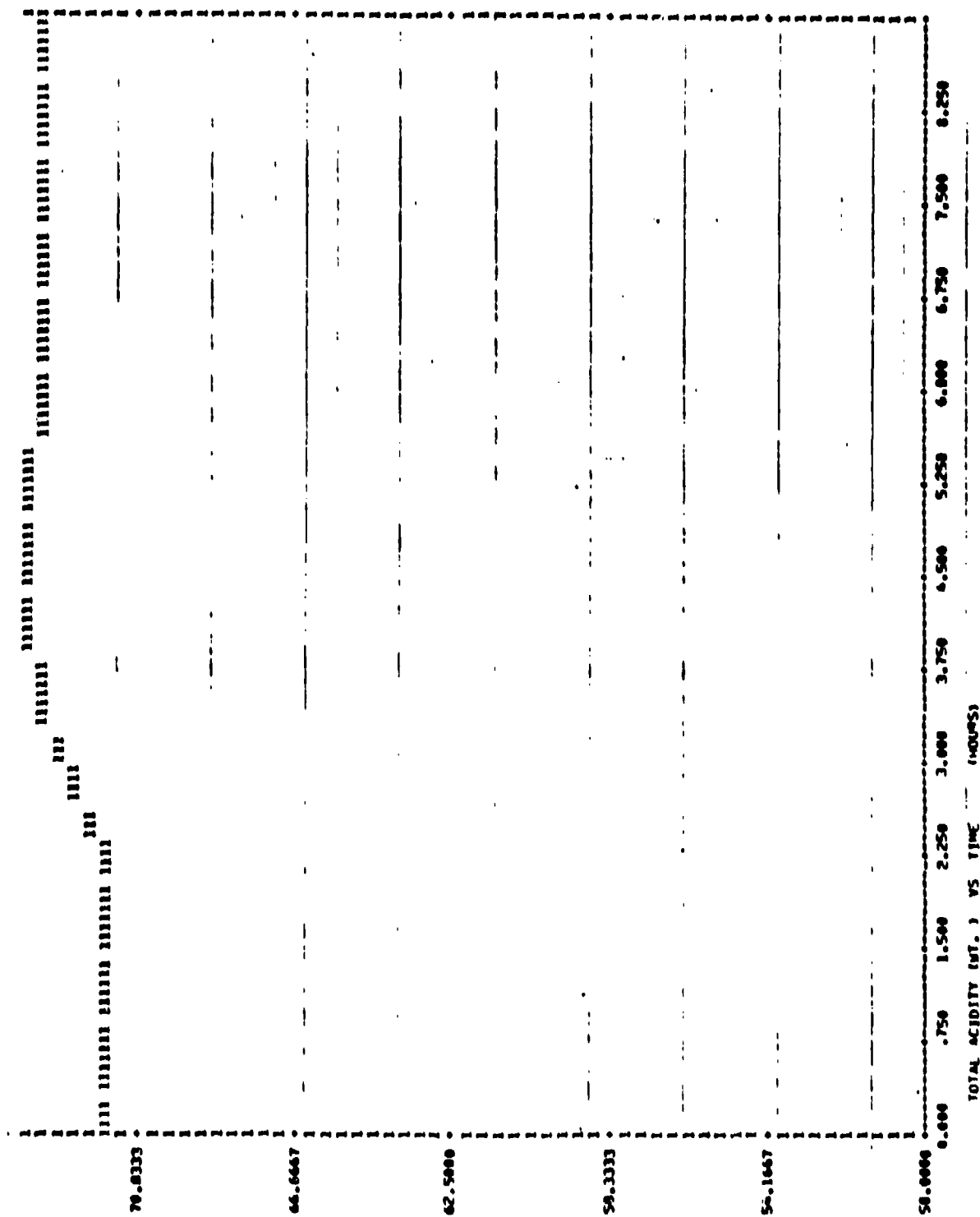
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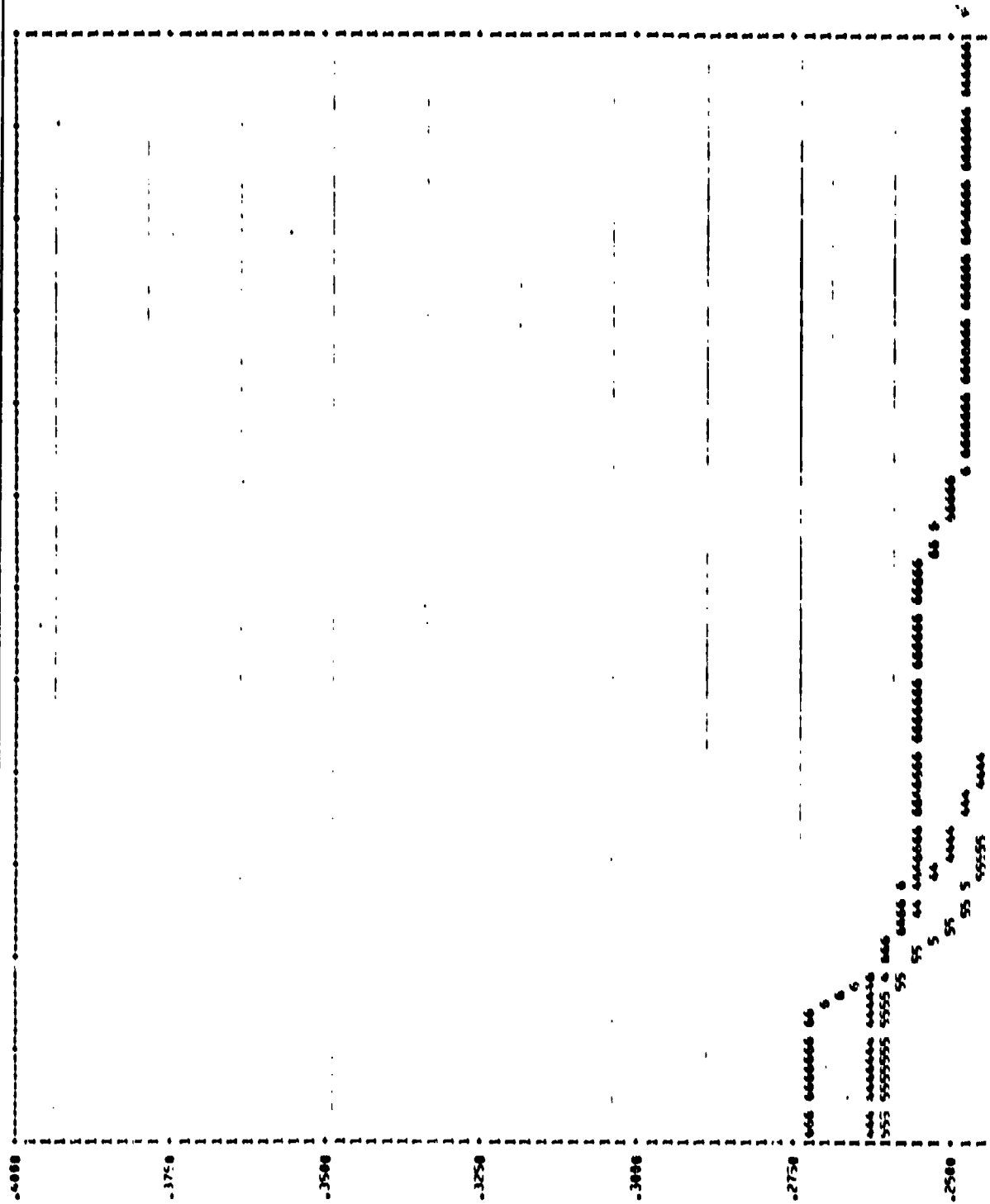
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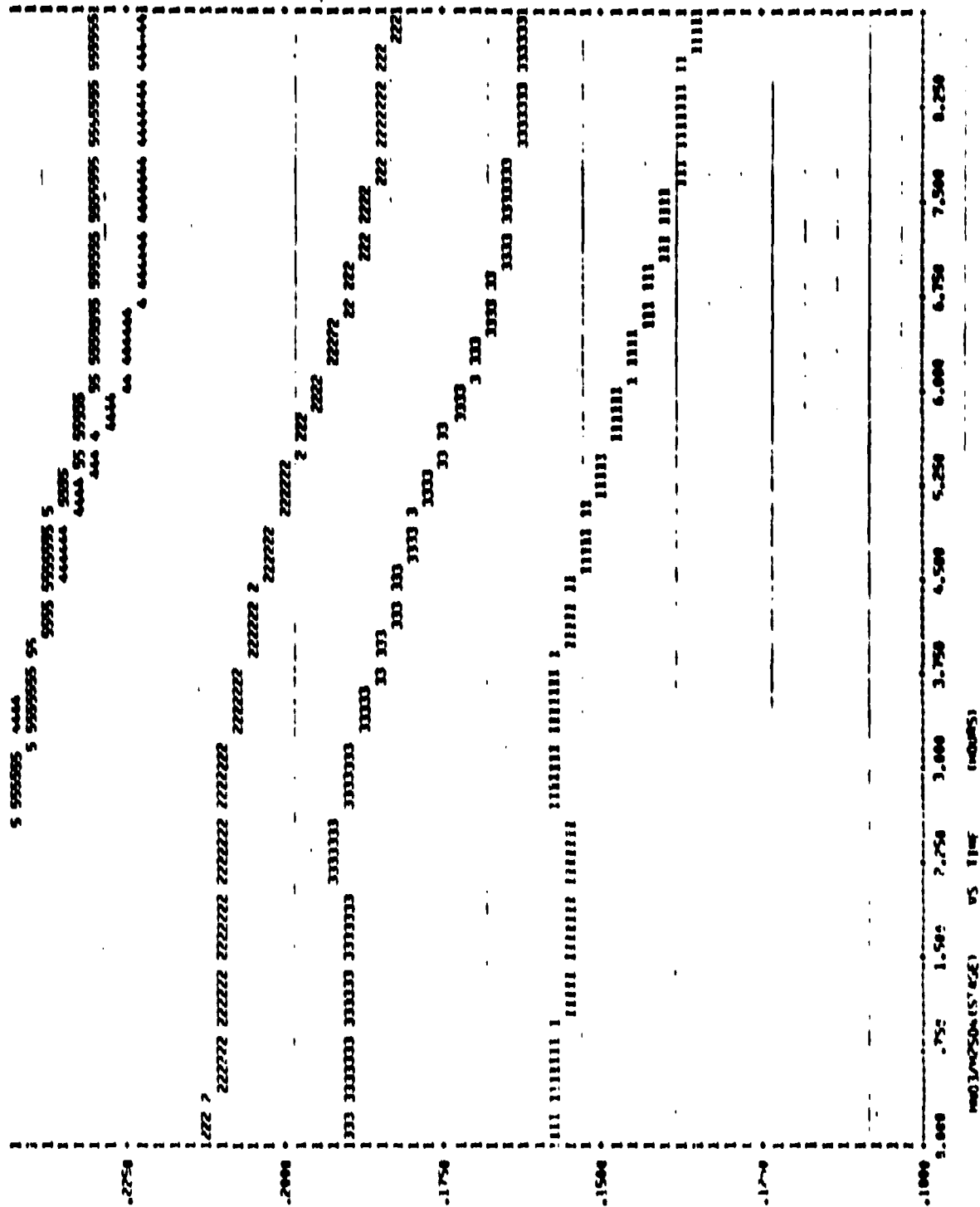
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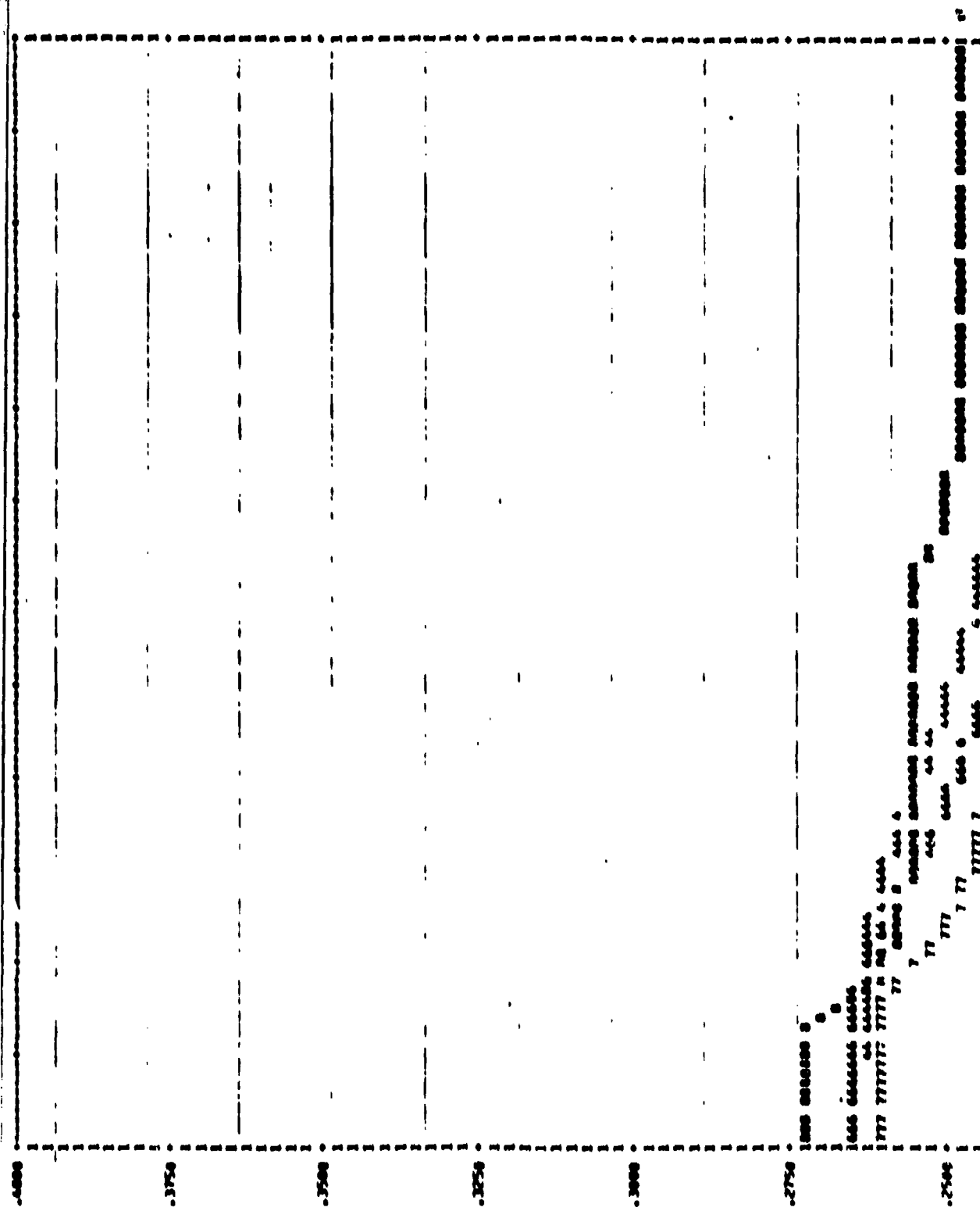


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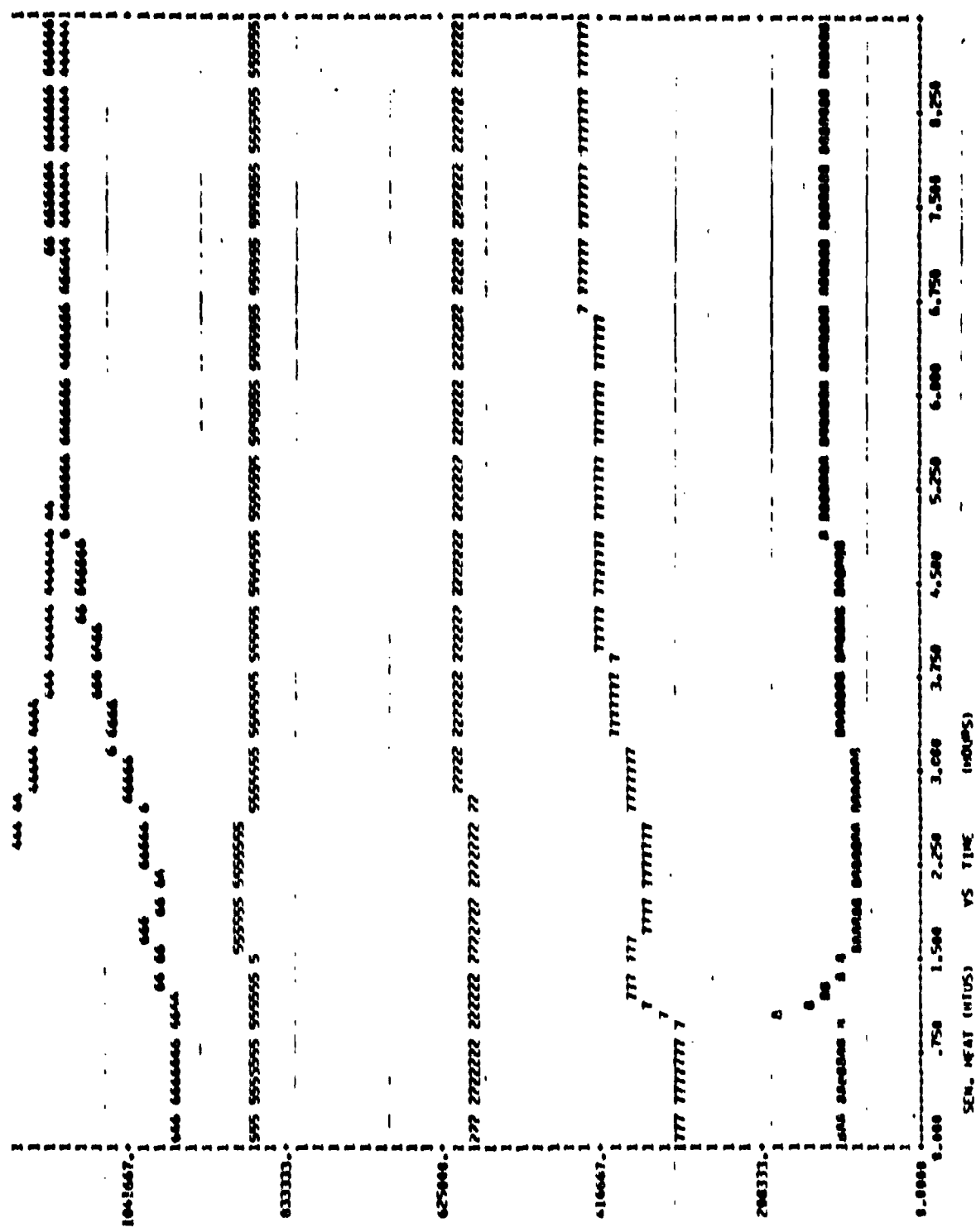
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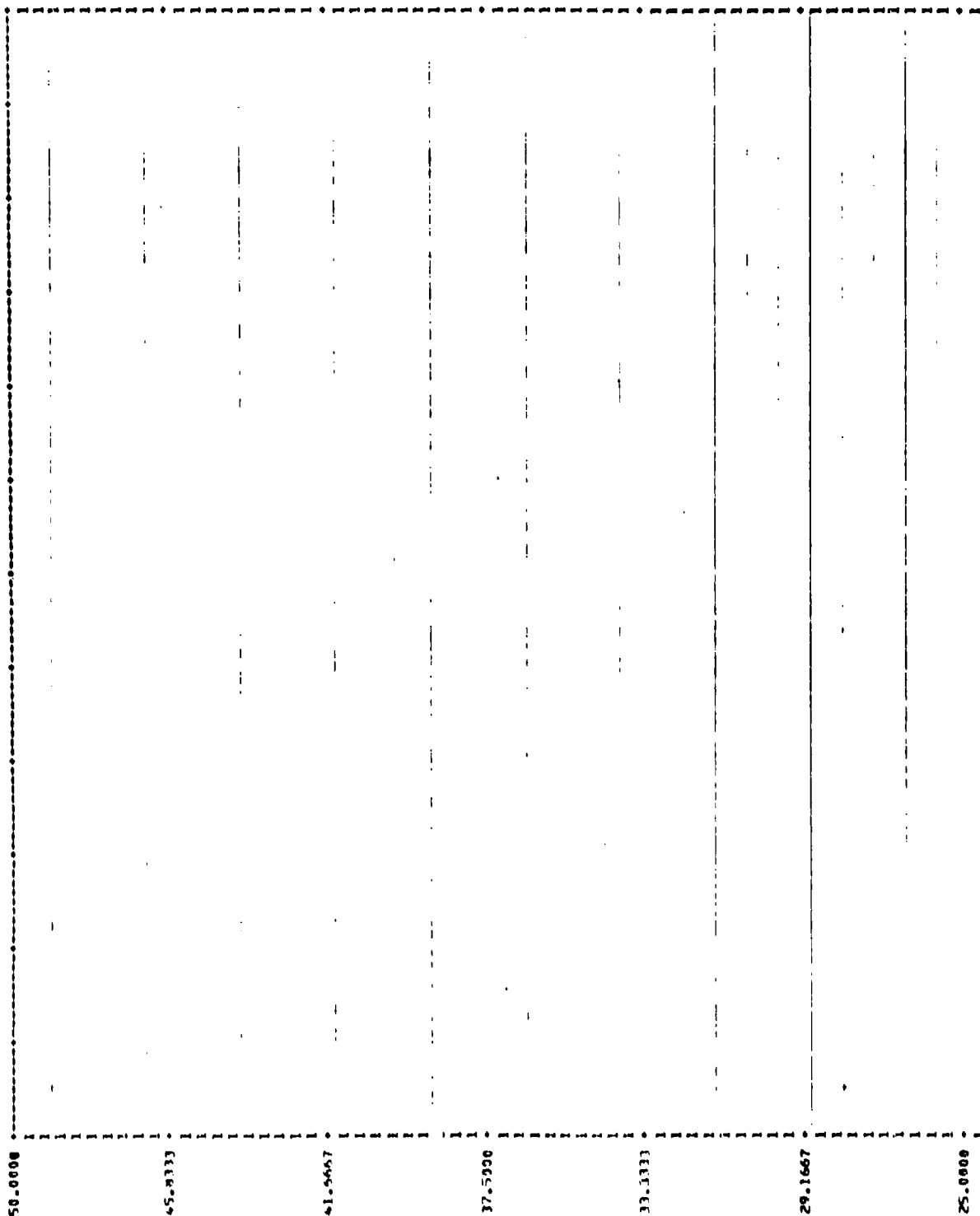
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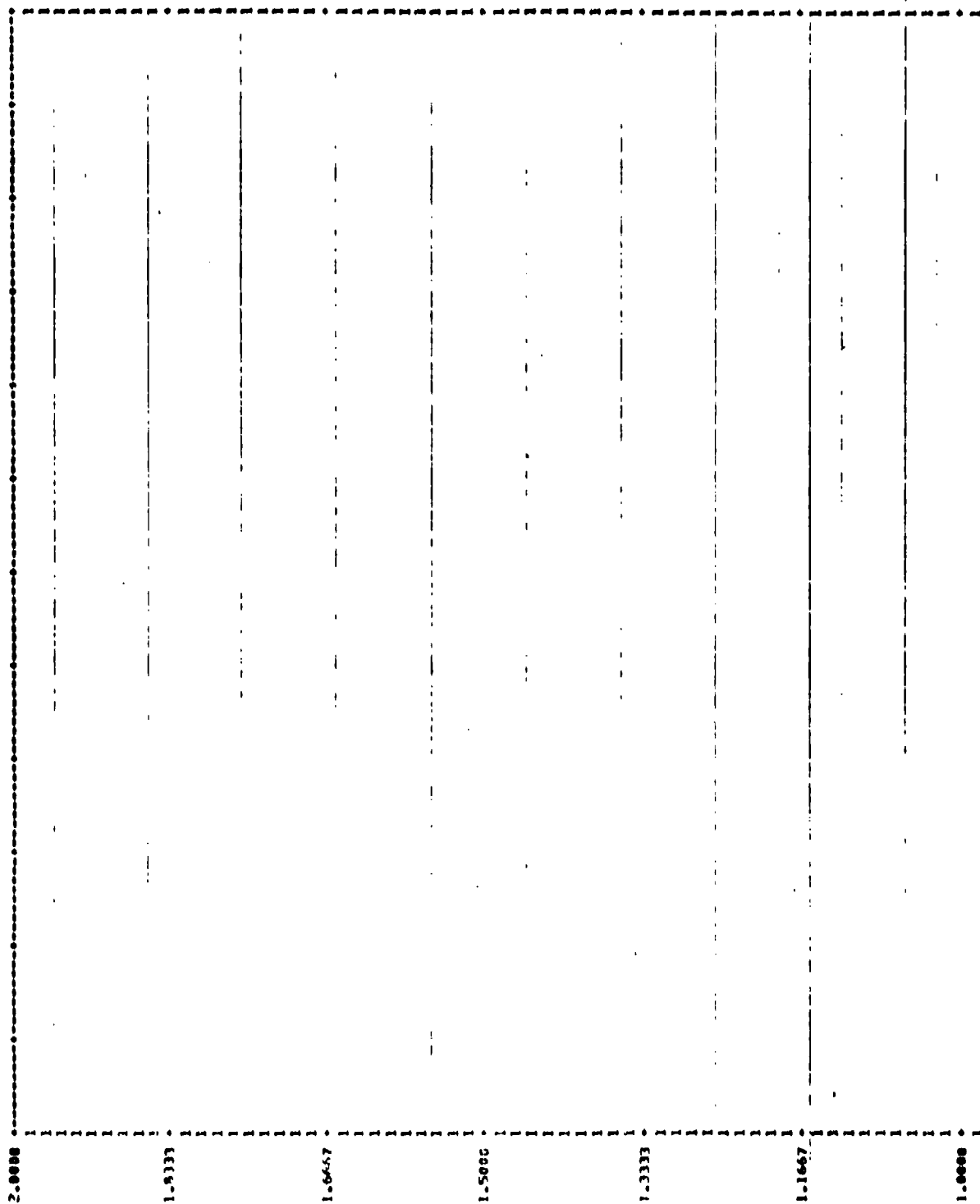
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0







20.0000

19.3331

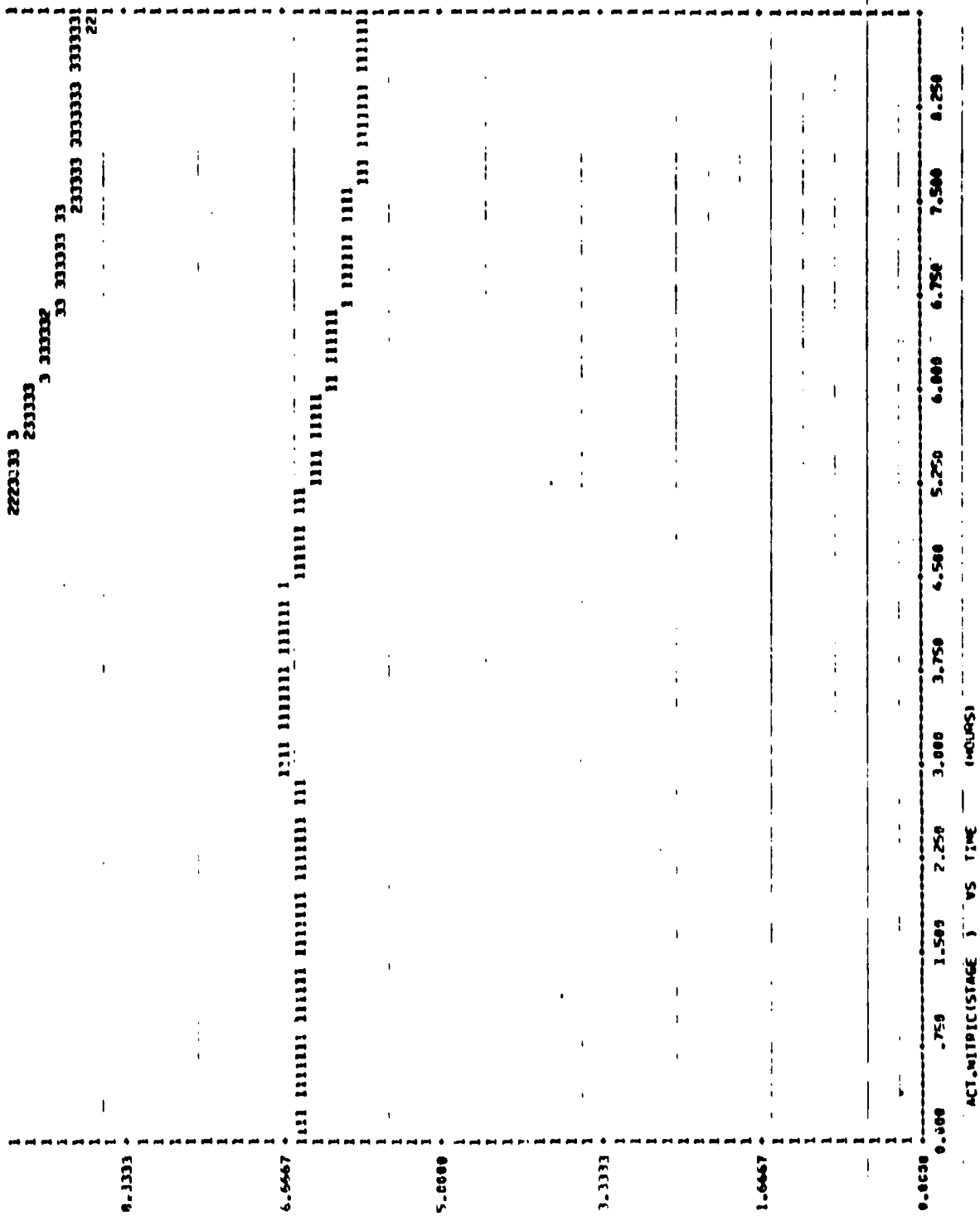
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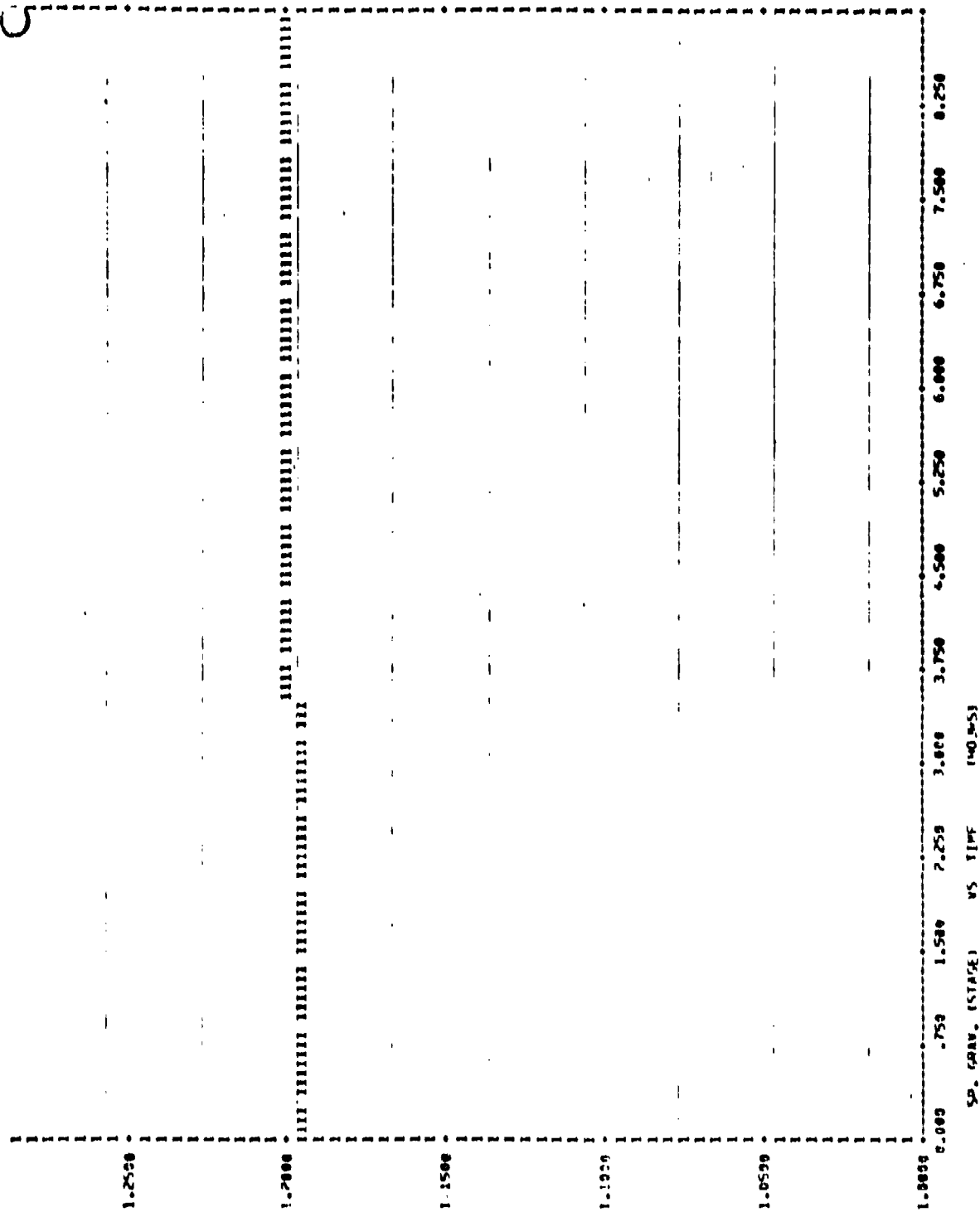
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1.3000

5



2.0000

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1.5000

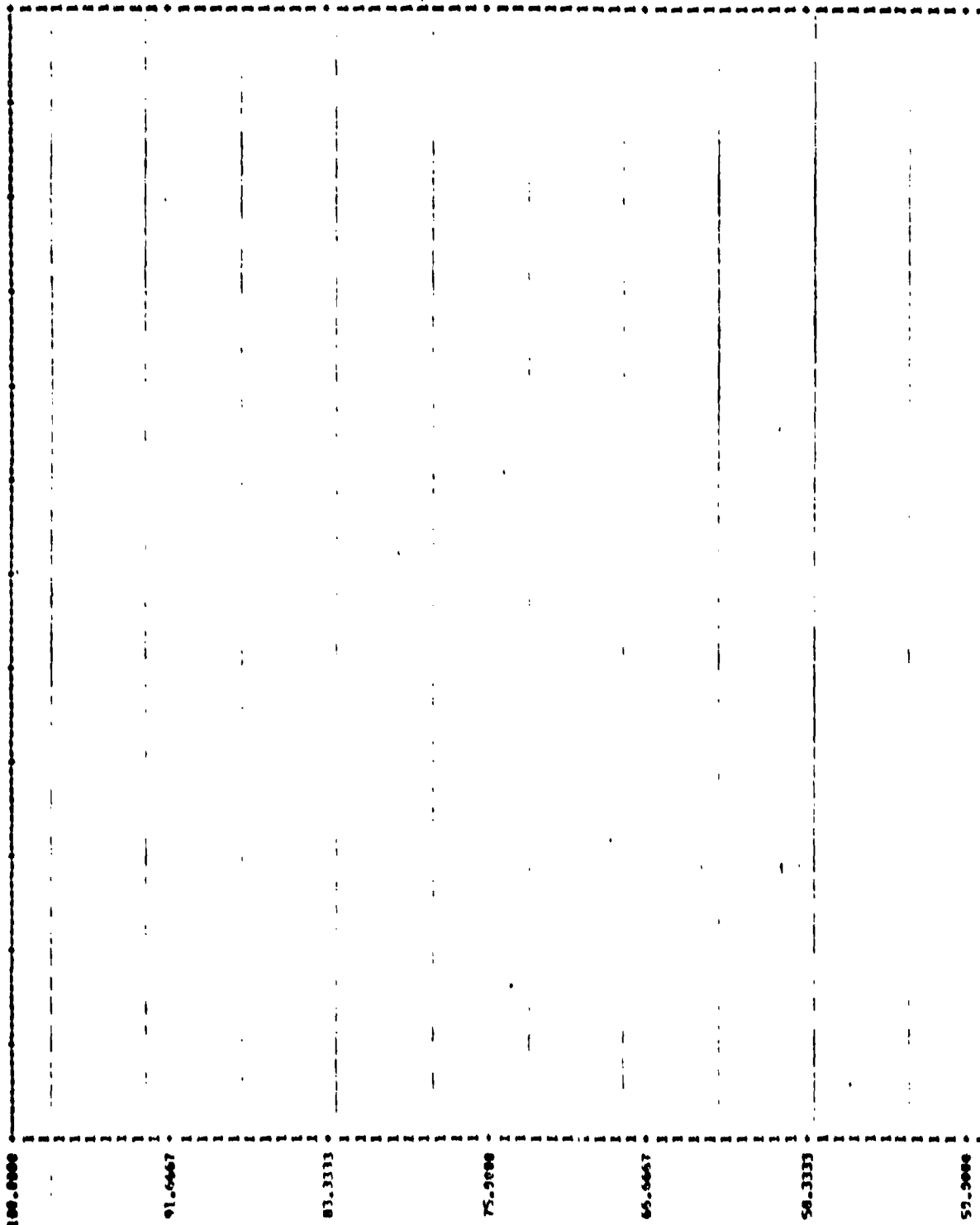
Q

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0.000	.750	1.500	2.250	3.000	3.750	4.500	5.250	6.000	6.750	7.500	8.250
SP. GRAY. (STAGE) VS TIME (HOURS)											

0

14167.	13331.	12500.	11667.	10833.	10000.0000
					8.000
					.750
					1.500
					2.250
					3.000
					3.750
					4.500
					5.250
					6.000
					6.750
					7.500
					8.250

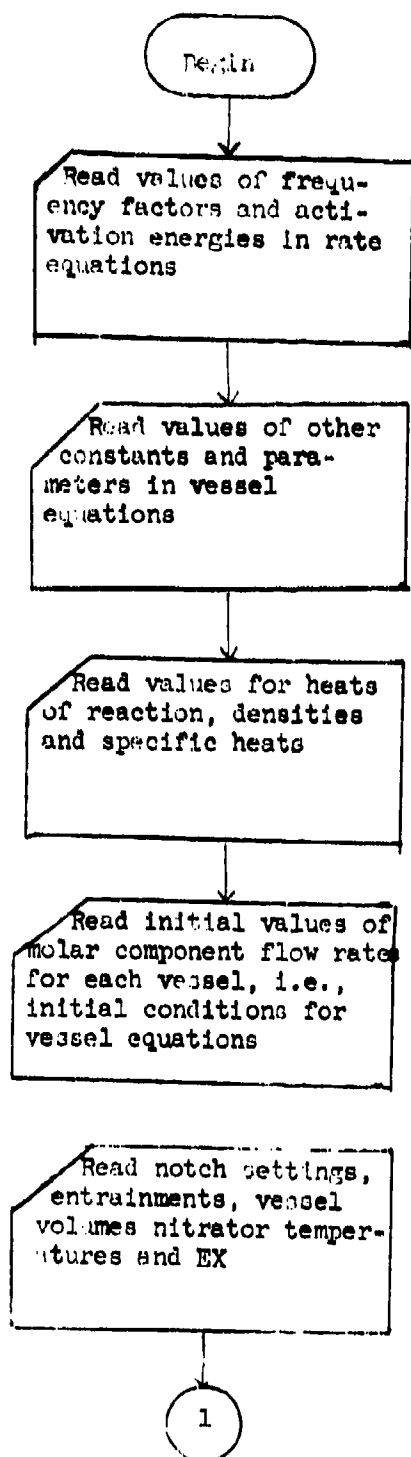
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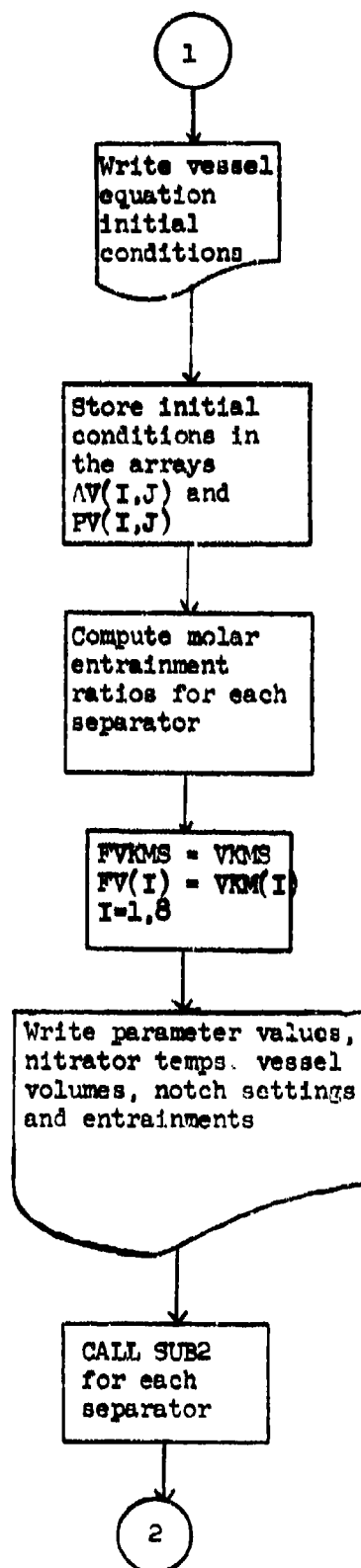


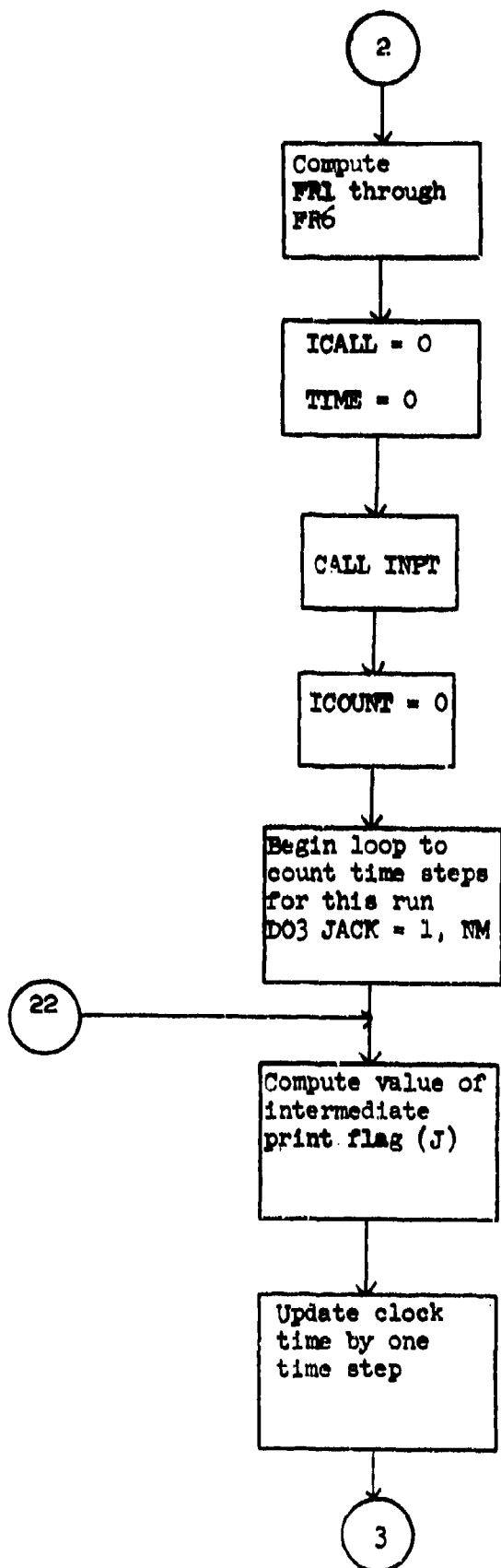
APPENDIX C

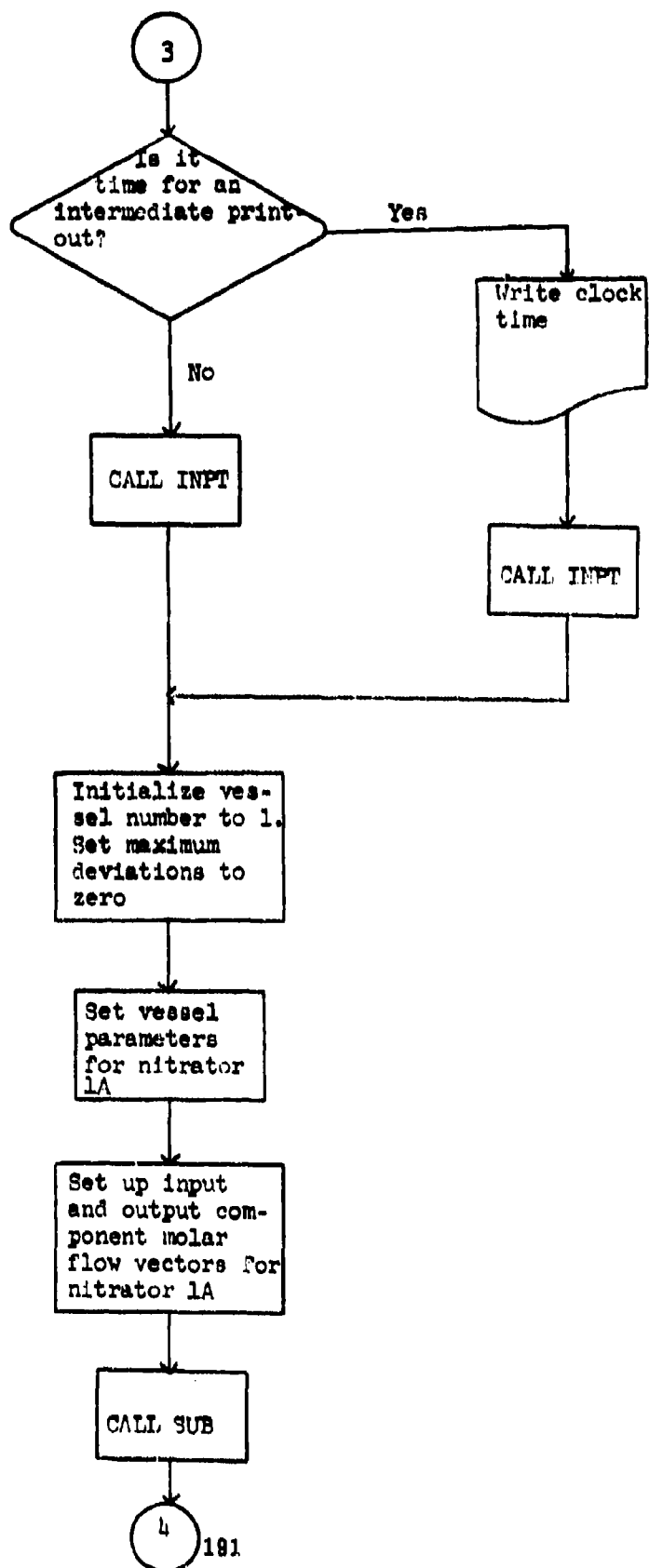
Dynamic Simulation--Program Flowchart

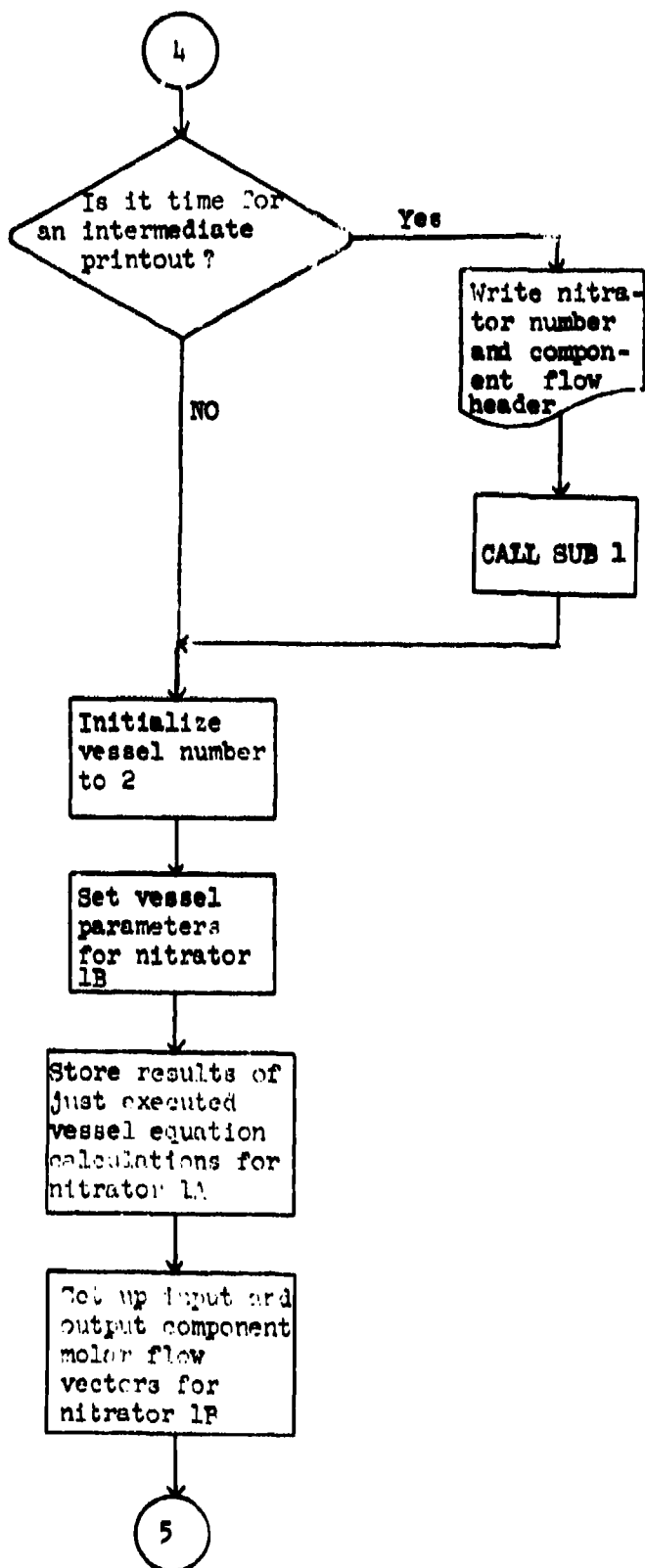
Main Program

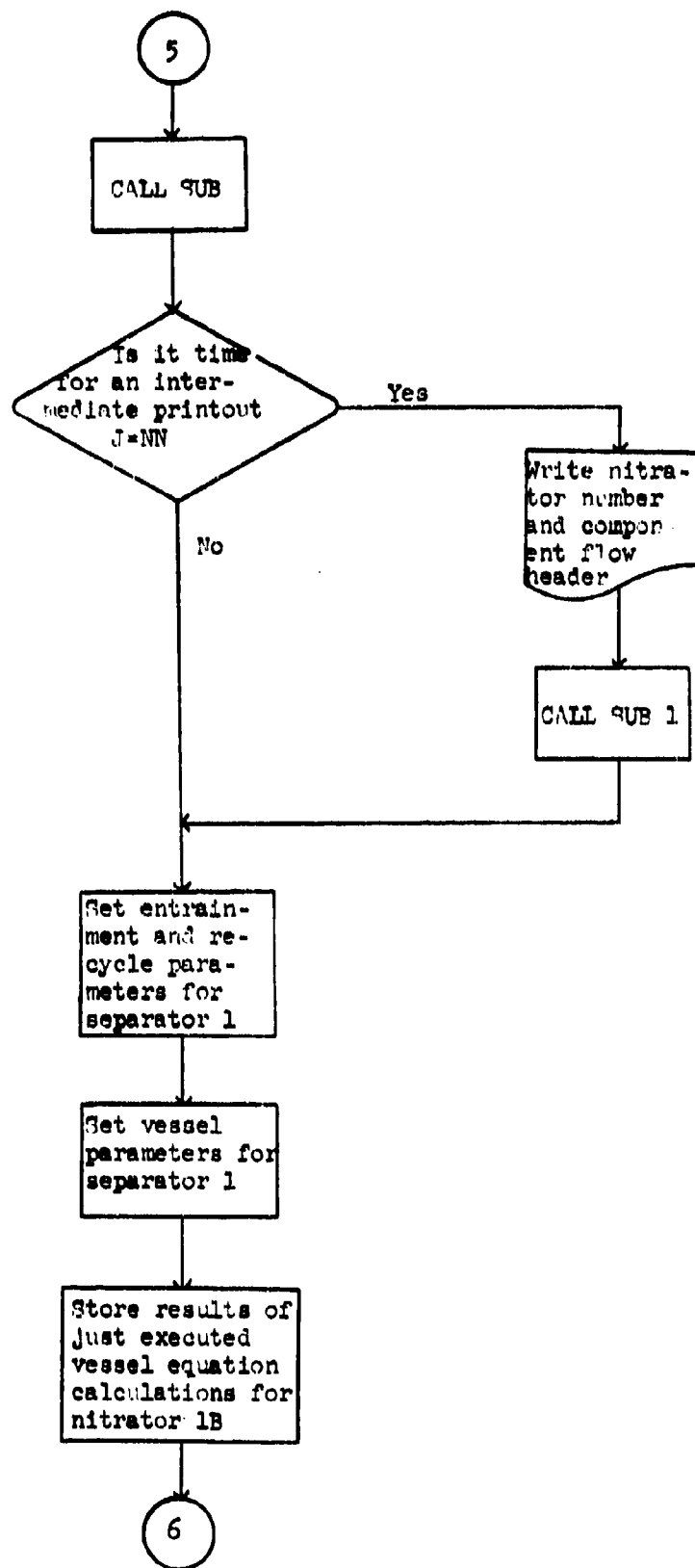


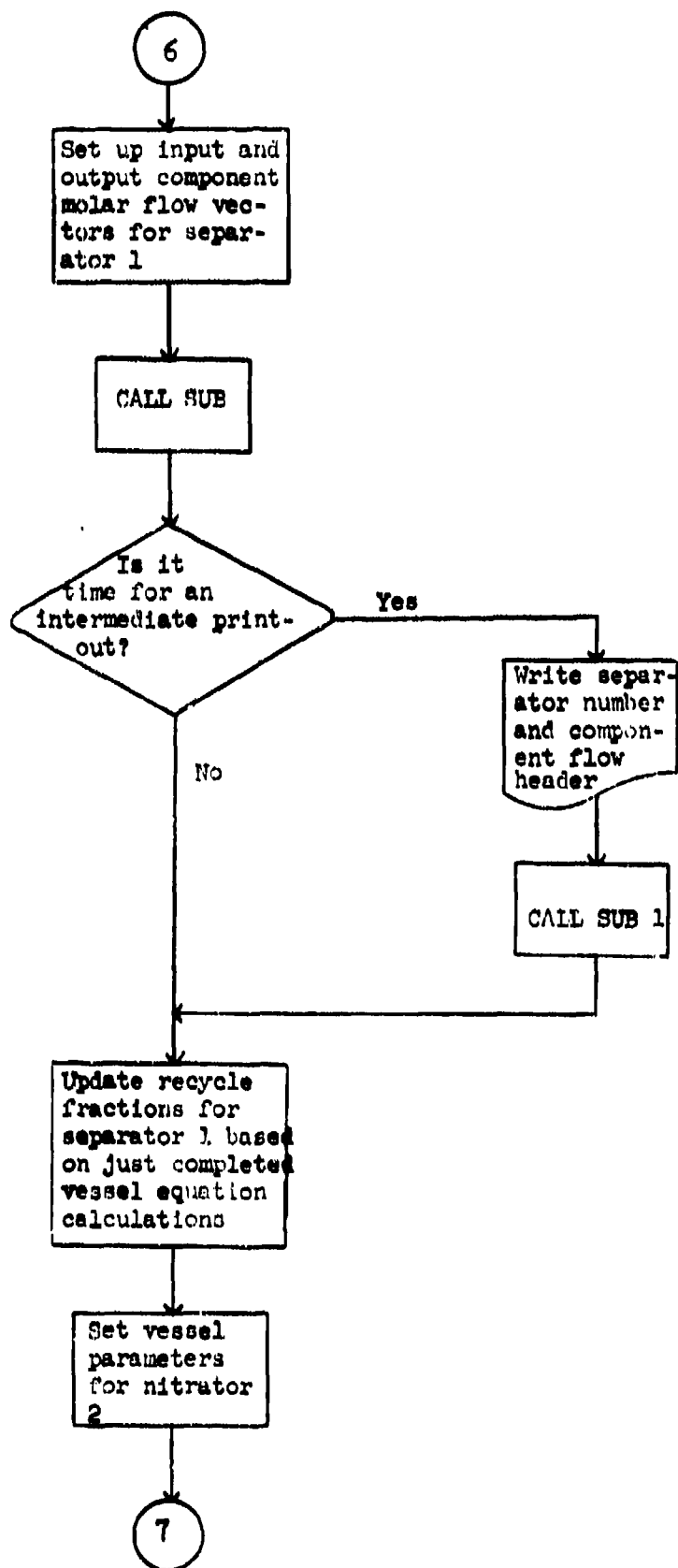


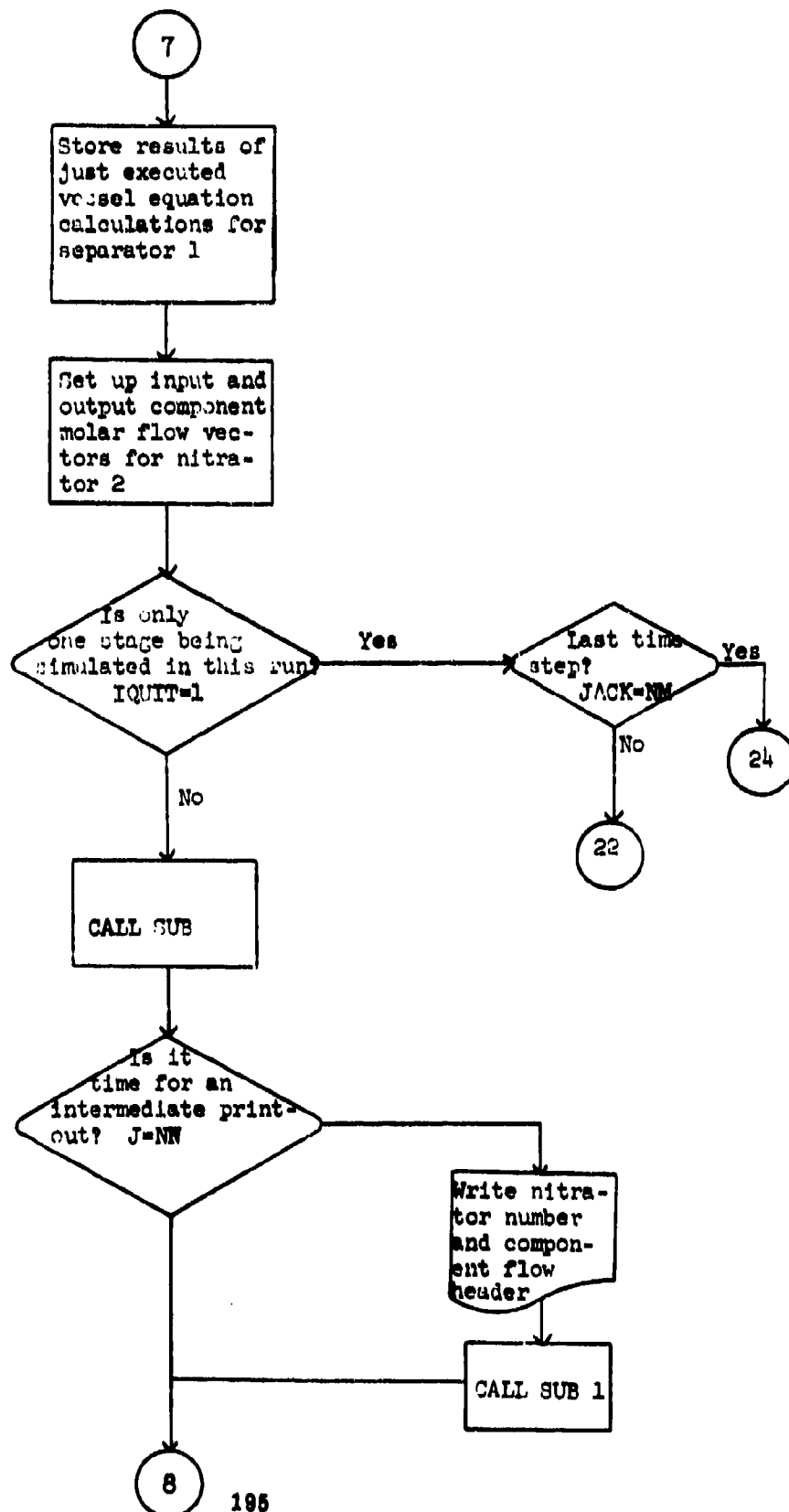


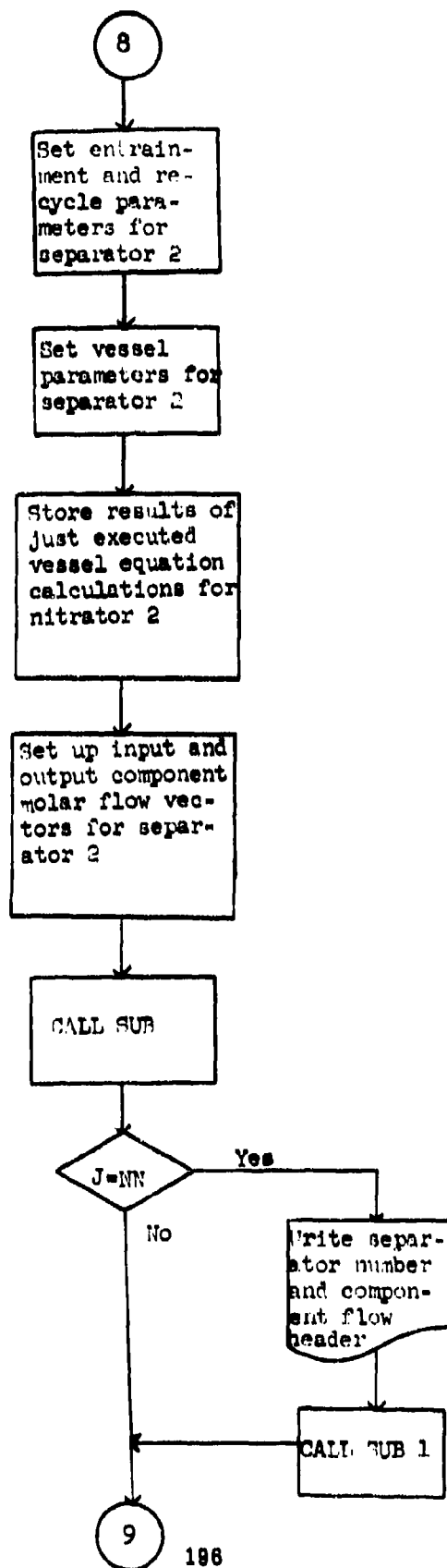


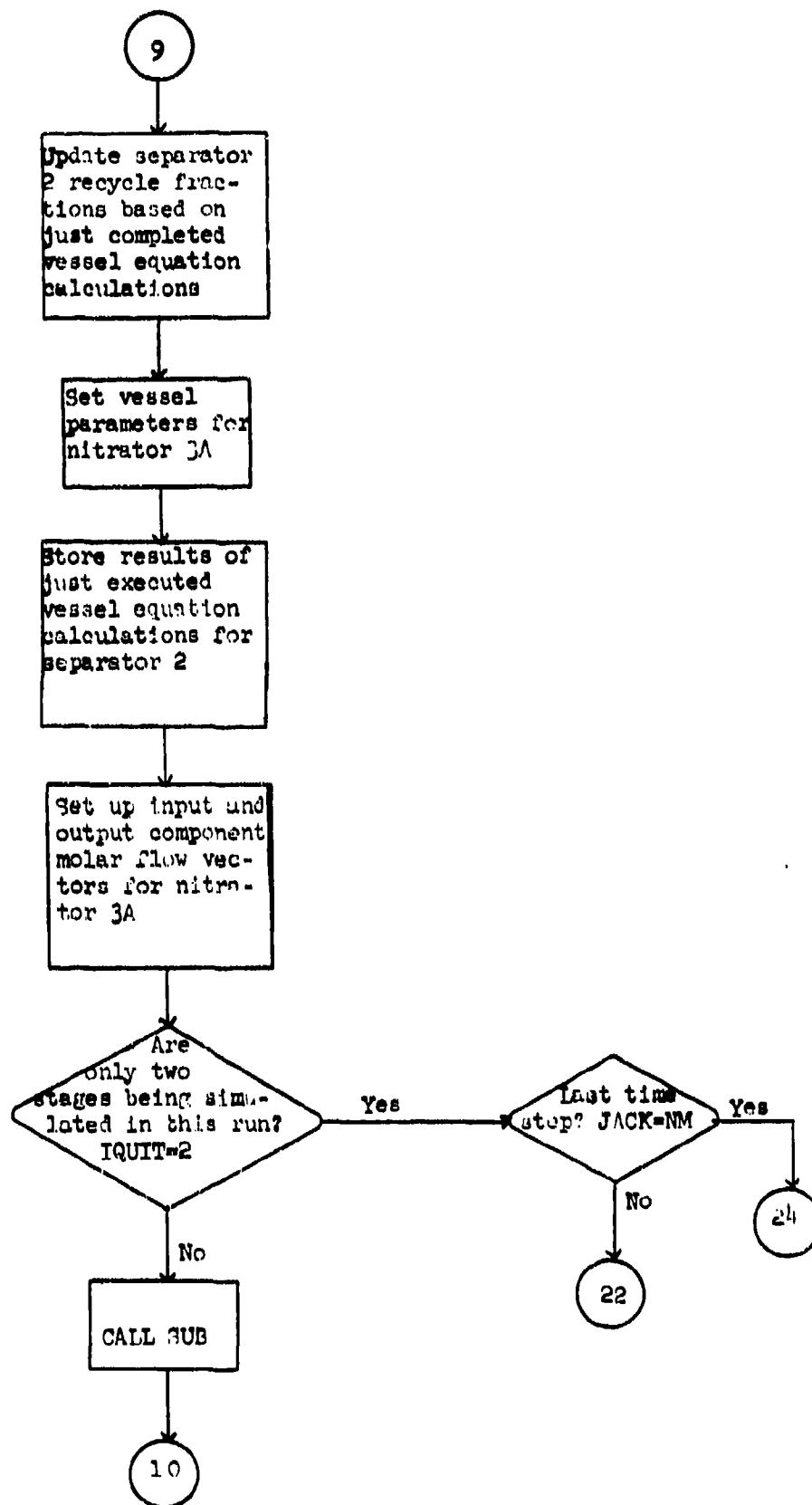


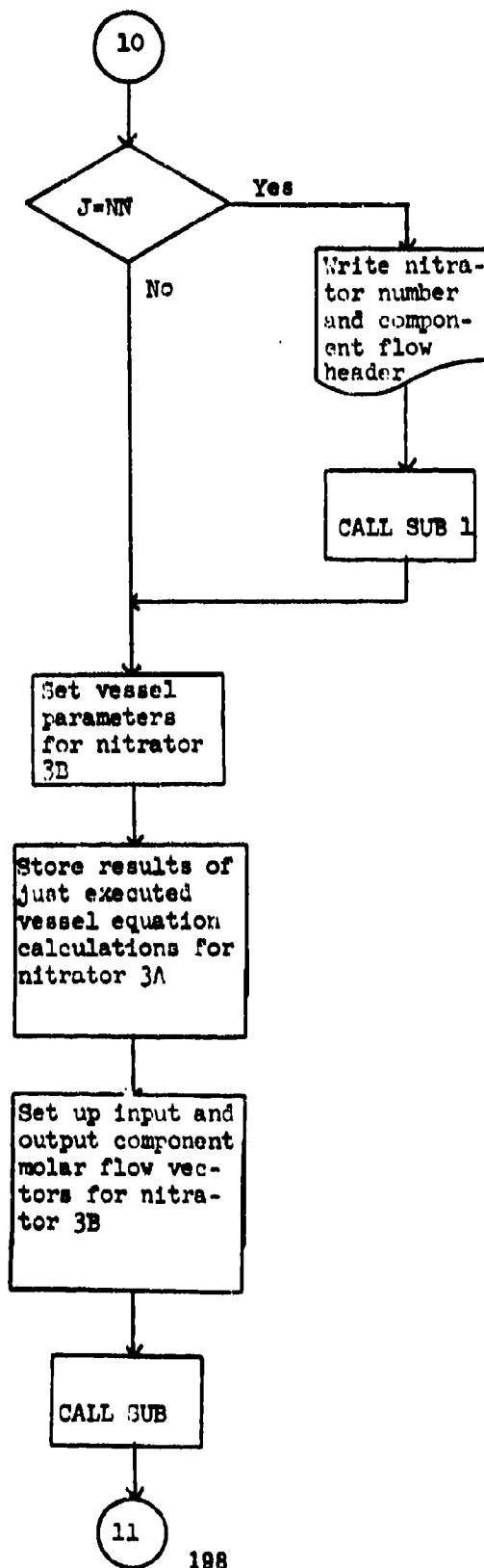


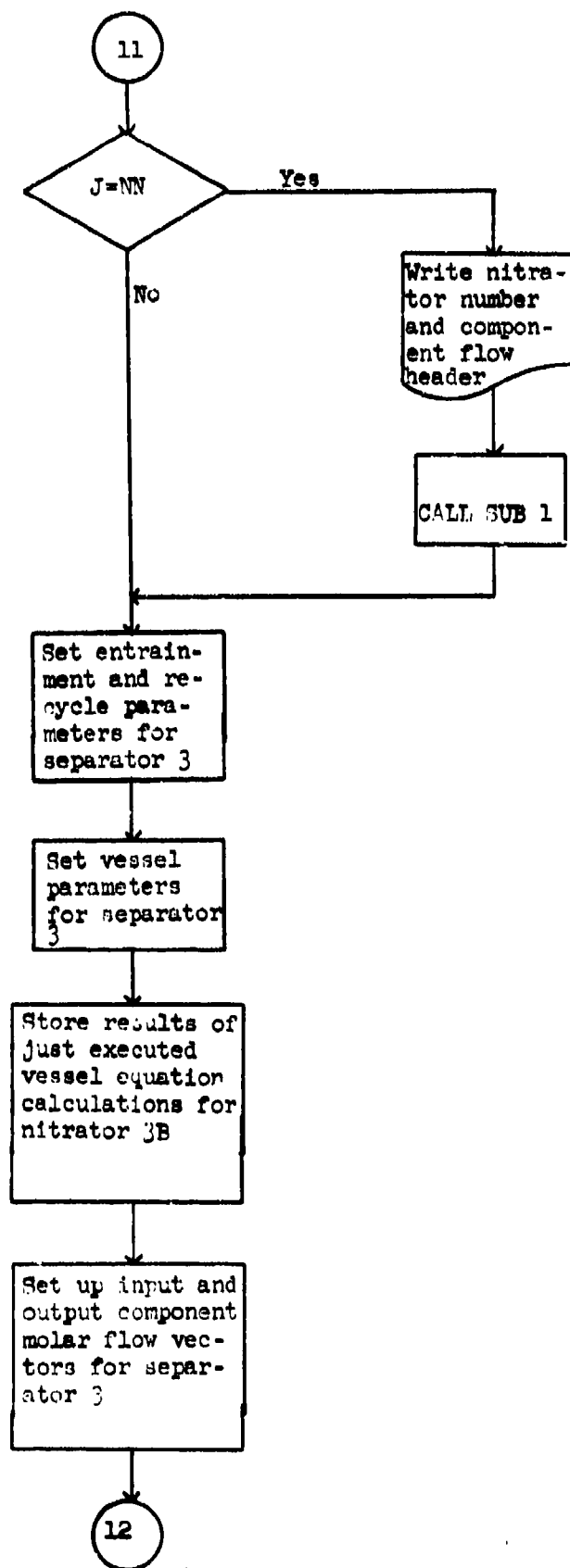


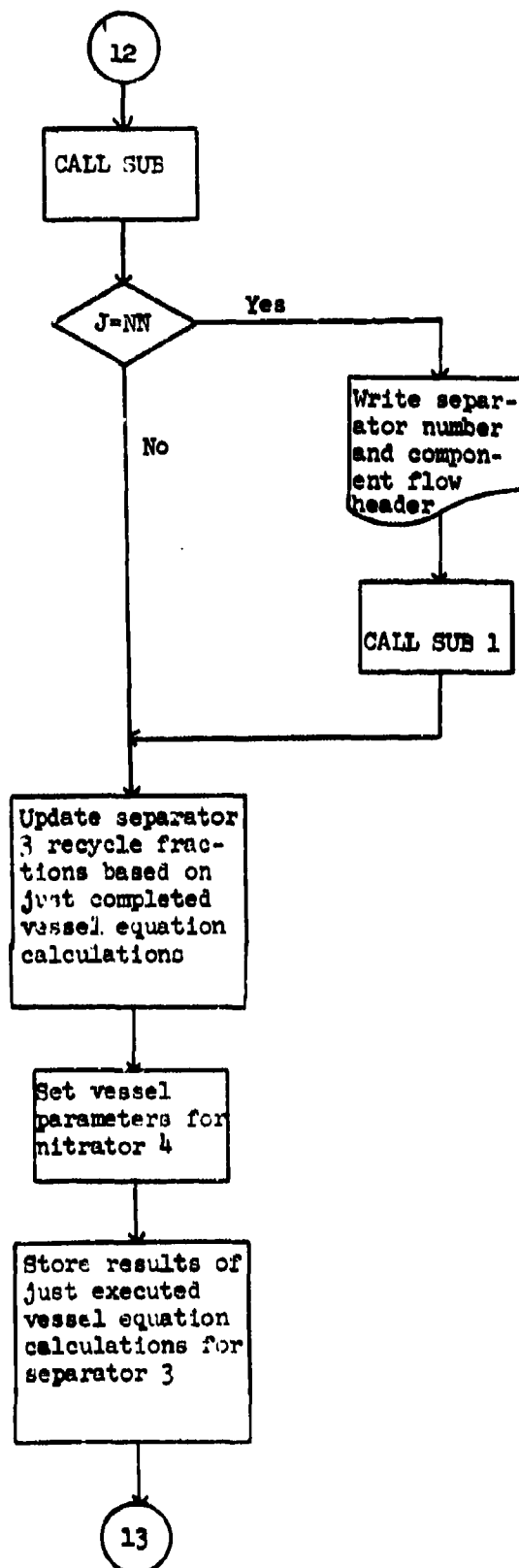


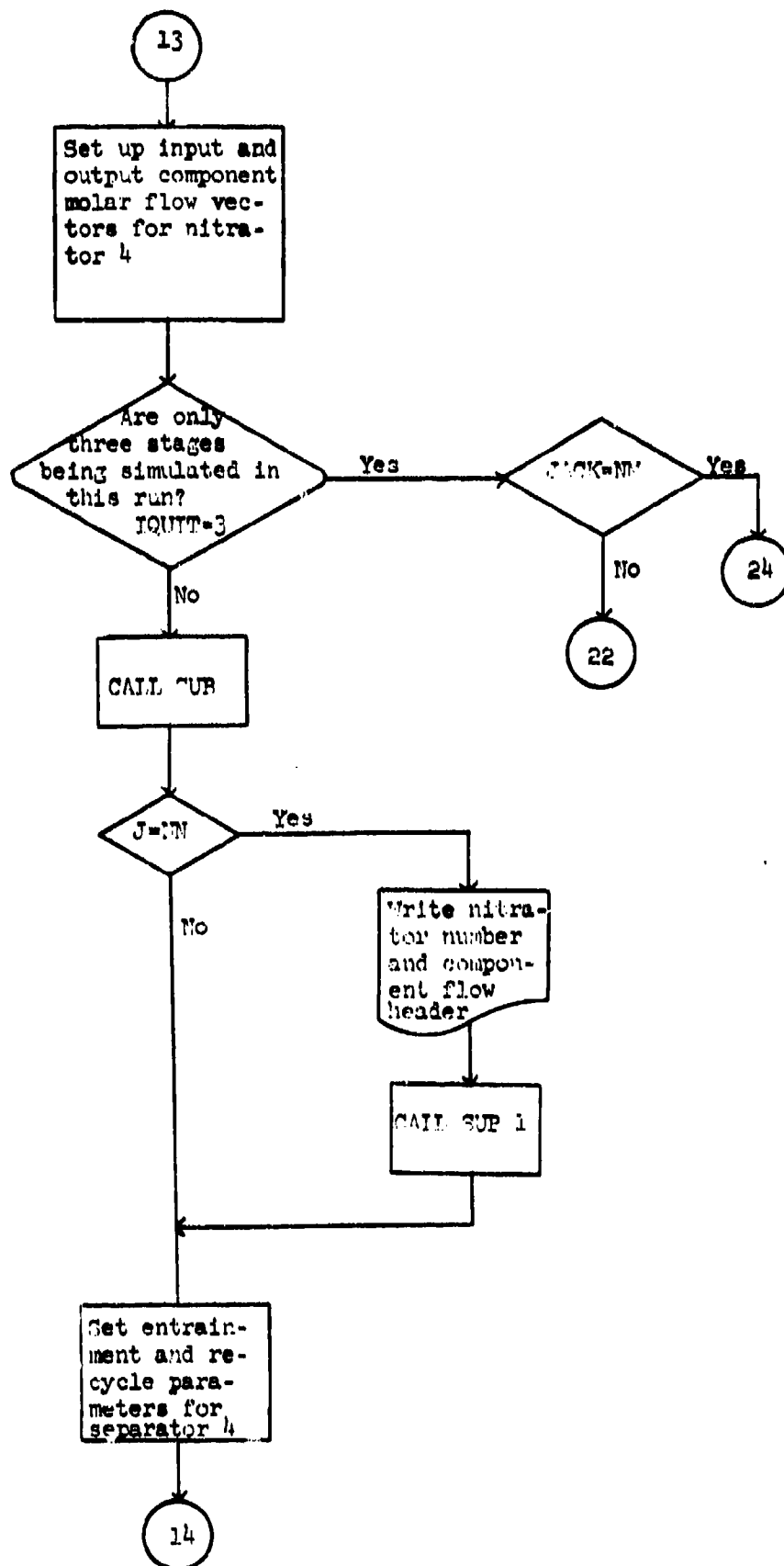


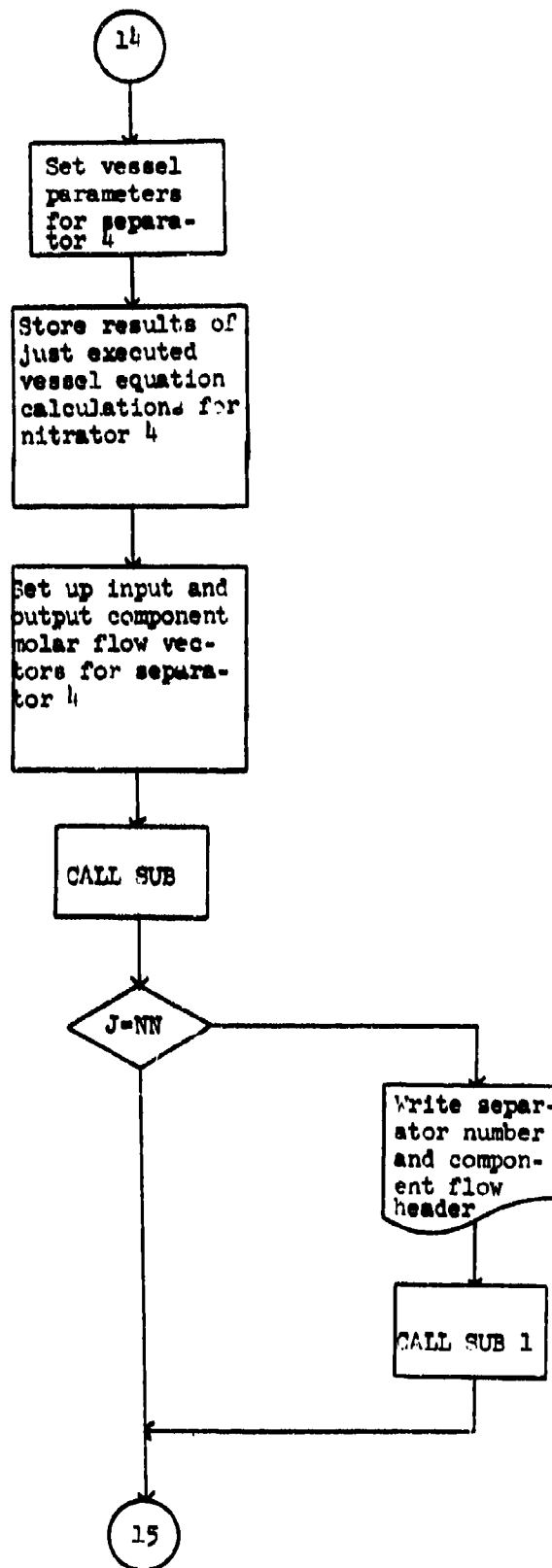


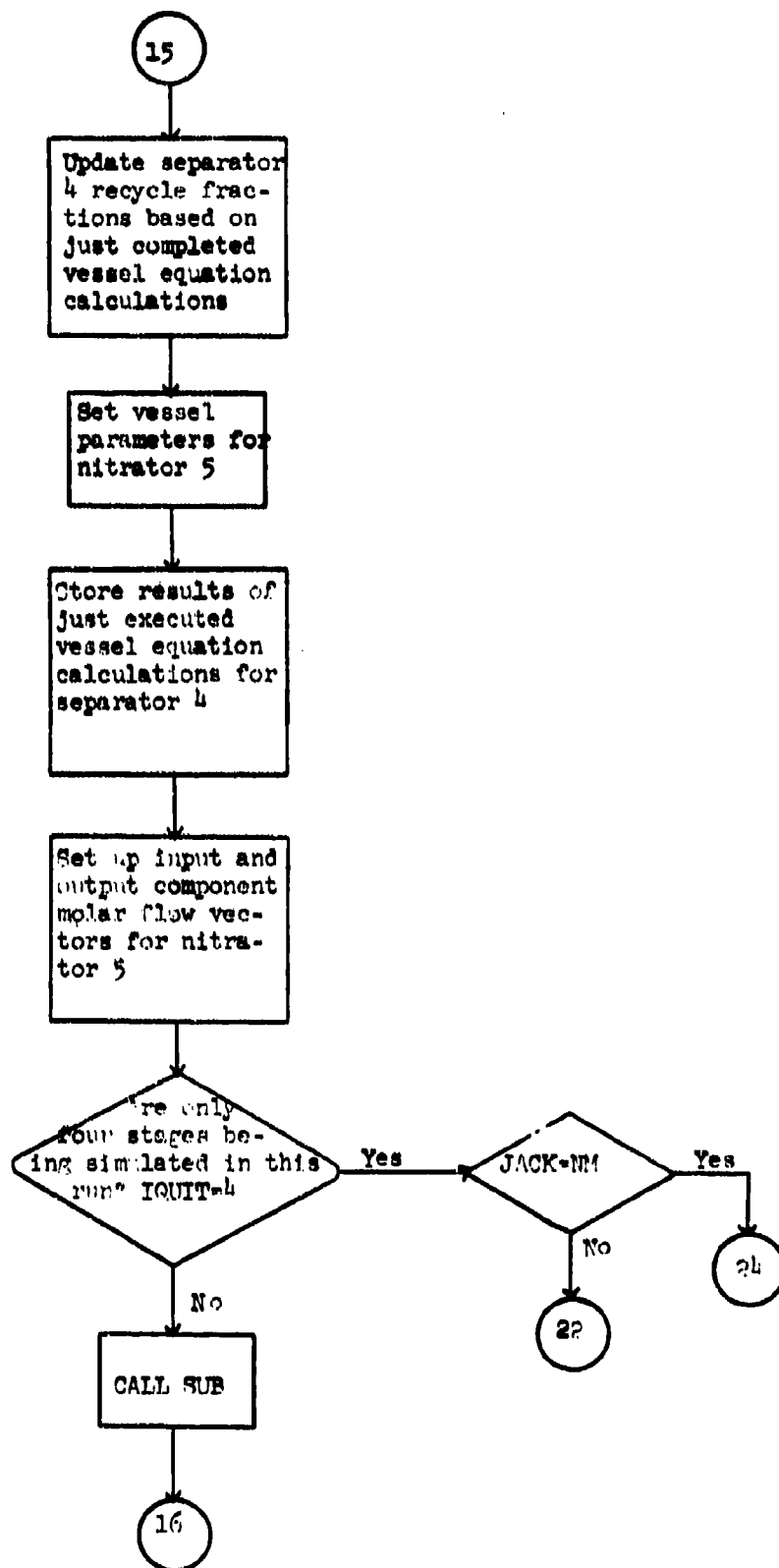


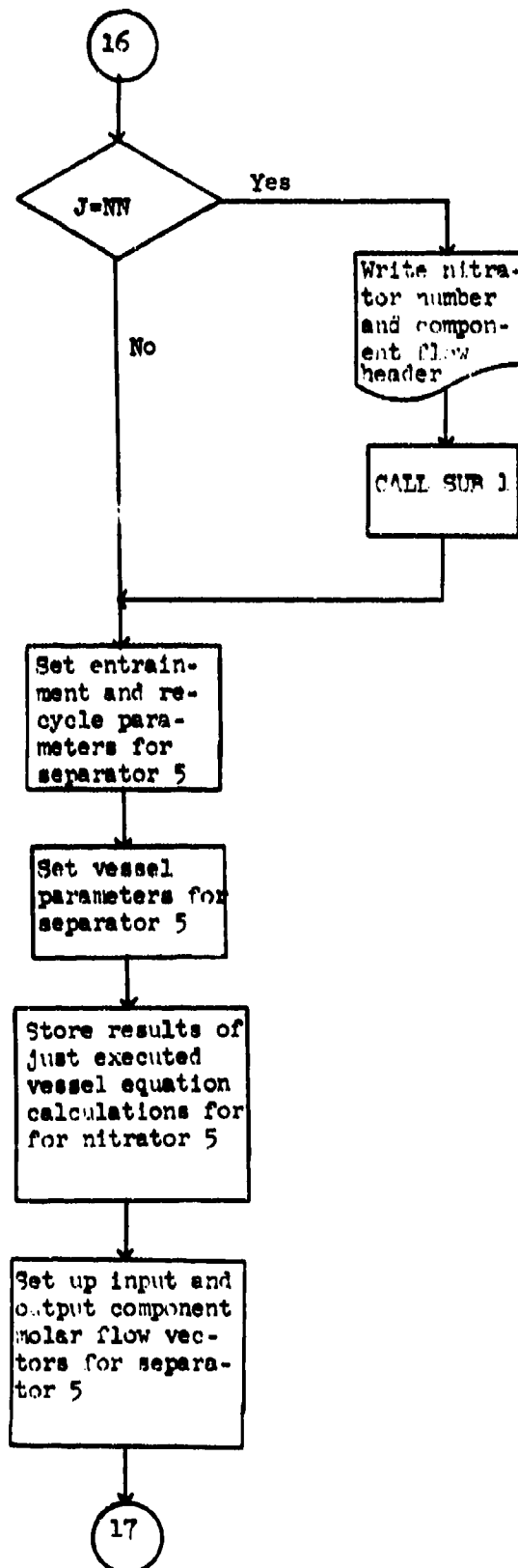


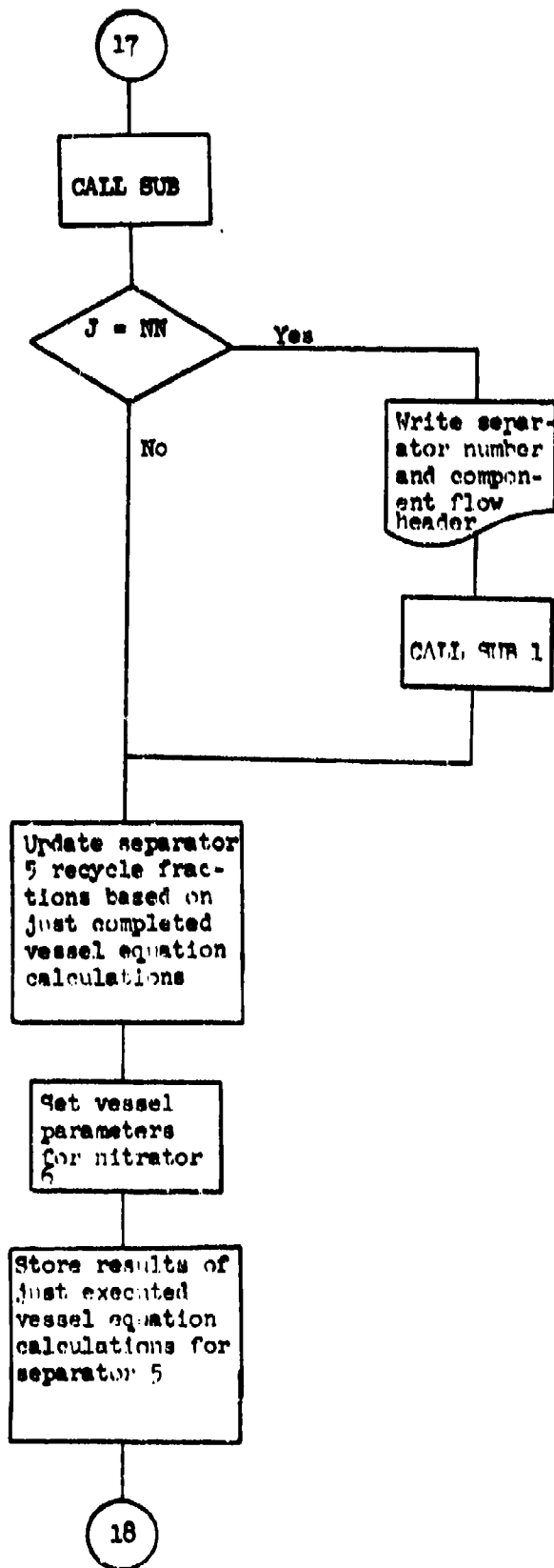


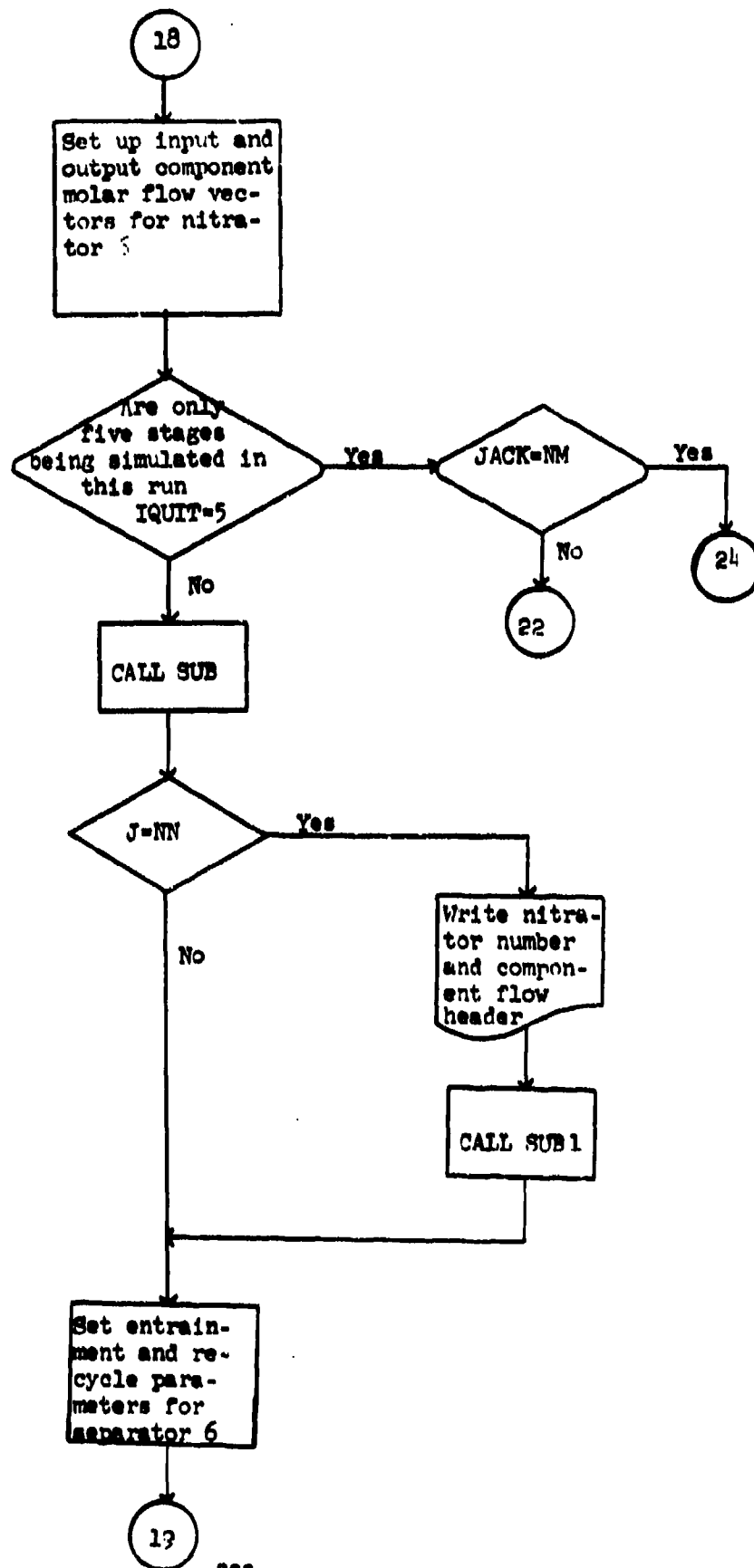


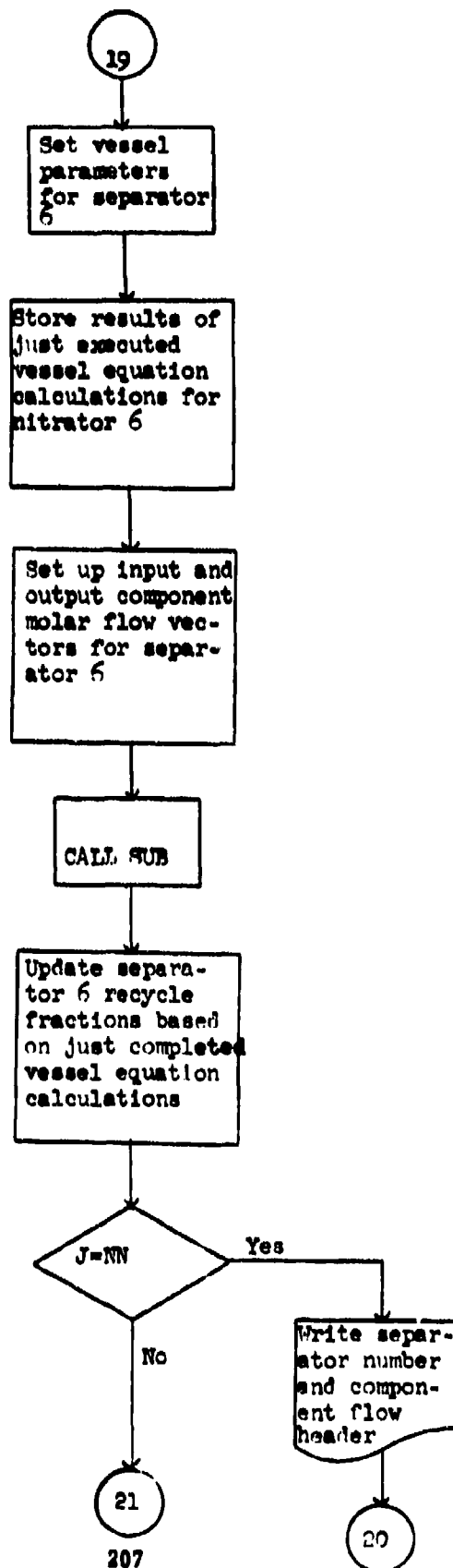












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CALL SUB 1

Write maximum percent
change in acid and
organic phase com-
ponents for this
iteration

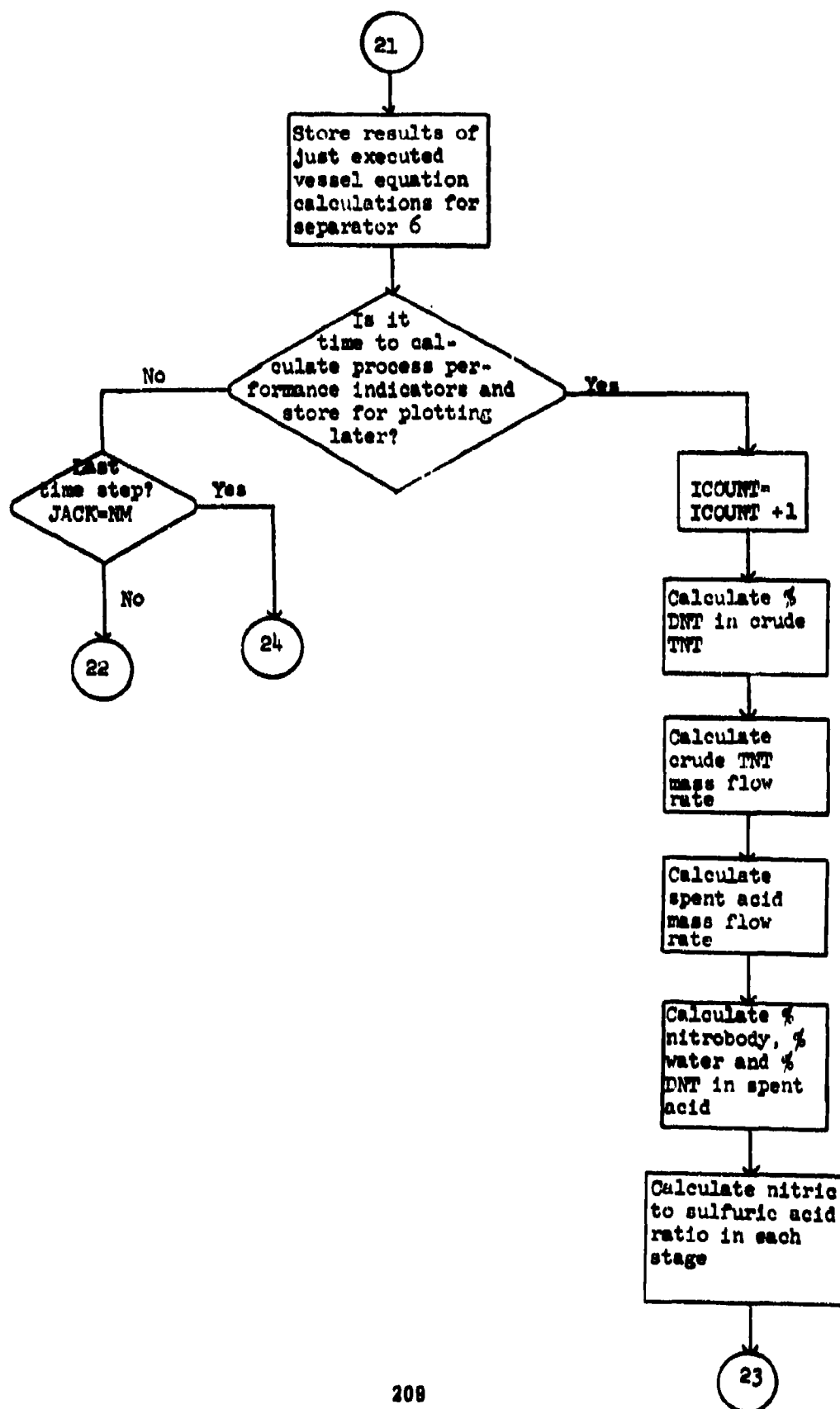
Write current
values of up-
dated recycle
fractions for
each separator

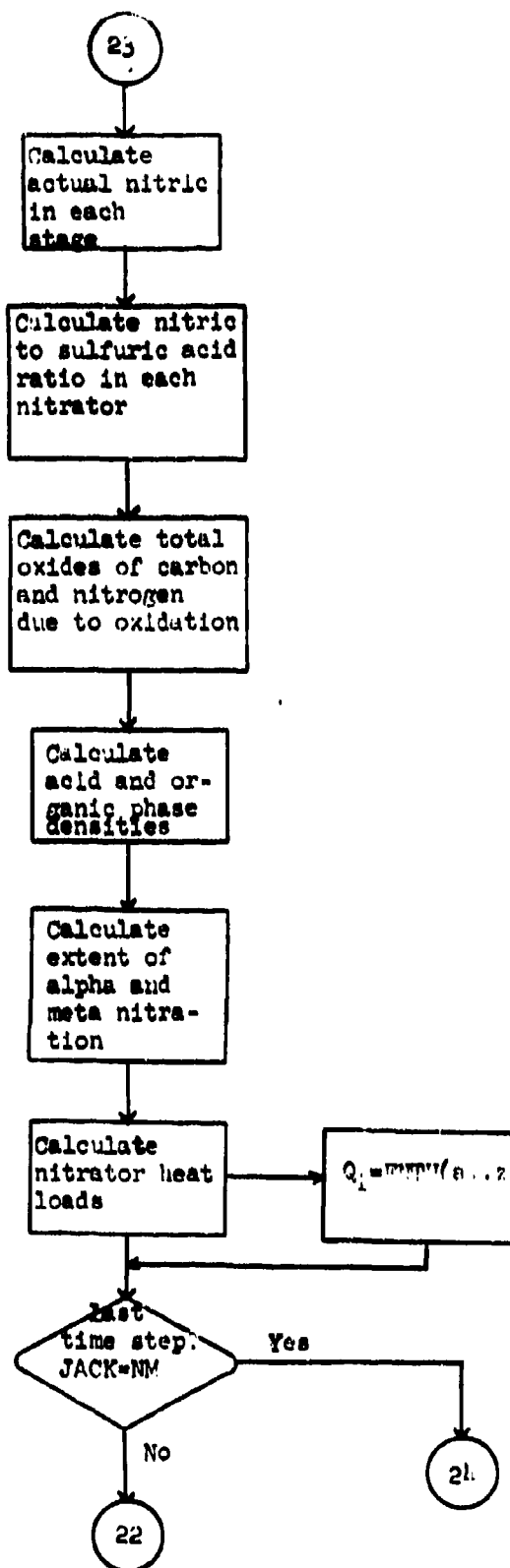
Compute molar
real stream com-
ponent flows
from ideal phase
flows

Compute total
mass and vol-
ume flows for
all real
streams

Write stream compon-
ent and flow data for
organic streams forward,
internal recycle and
external recycle for
each stage

21





24

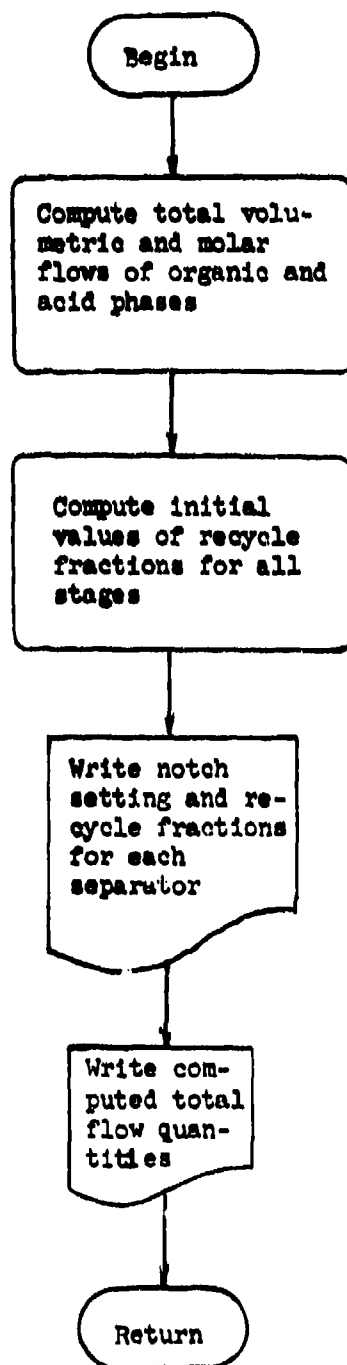
Write Process performance indicator tables

Call plotting subroutines

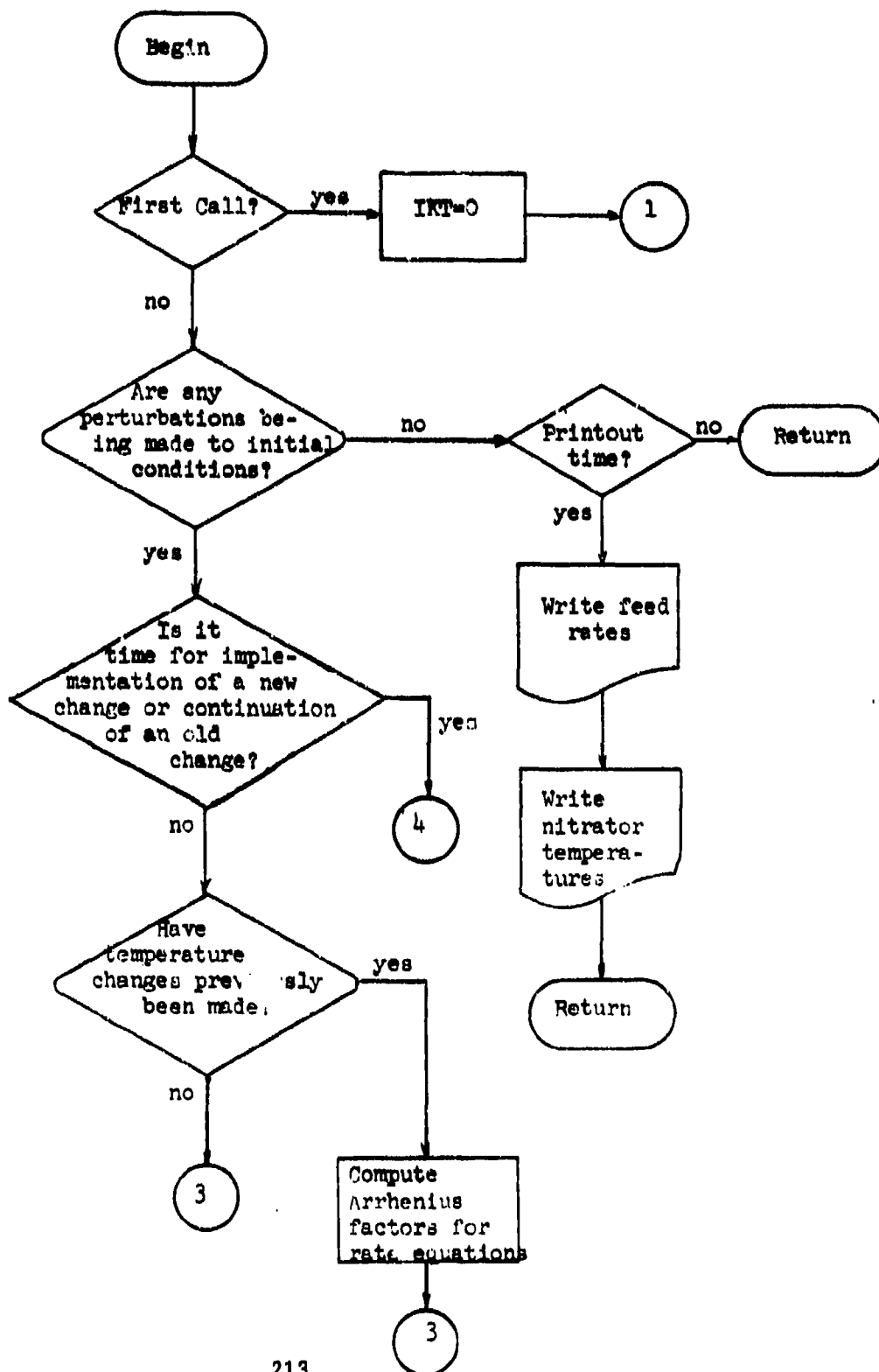
Plot process performance indicators vs. time

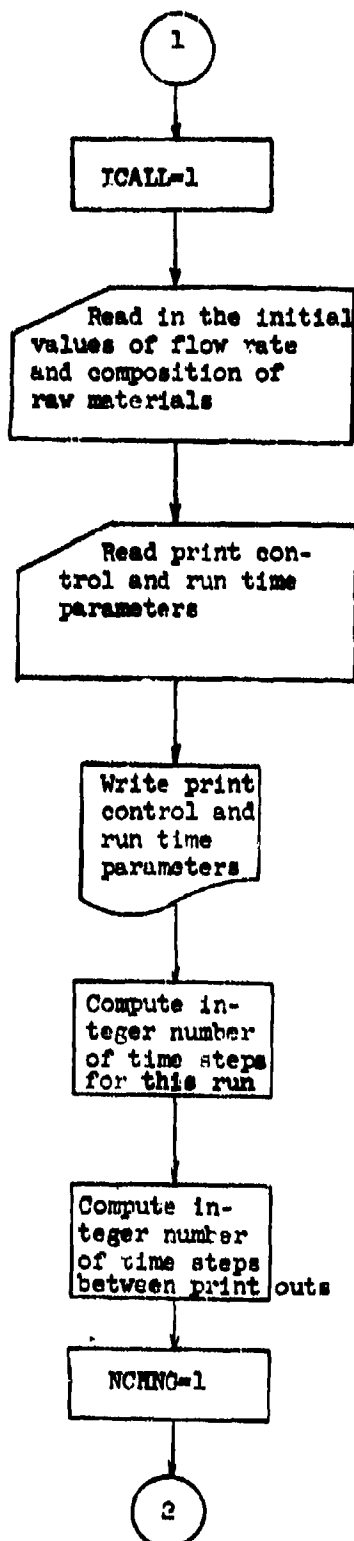
STOP

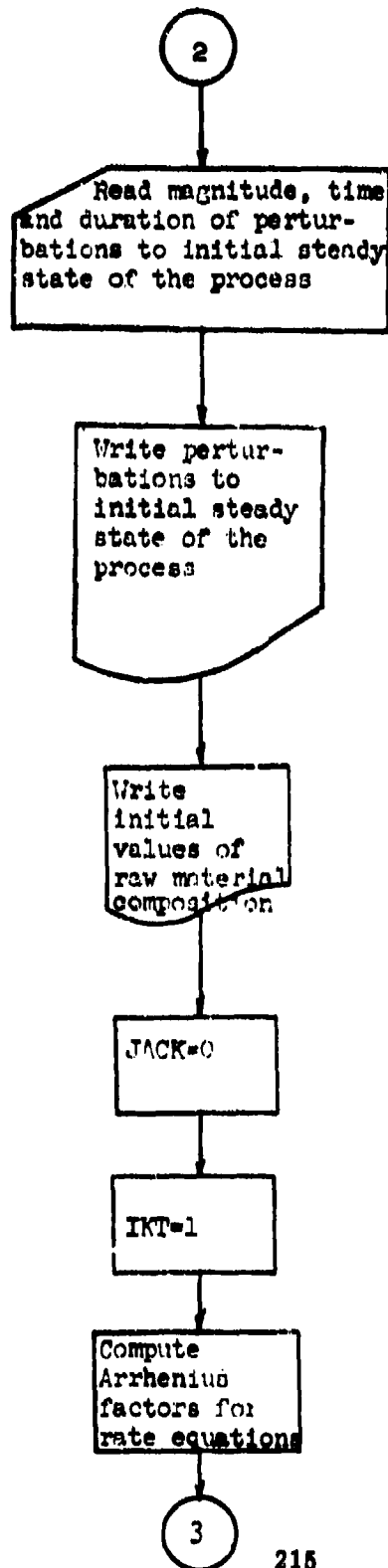
Subroutine SUB2

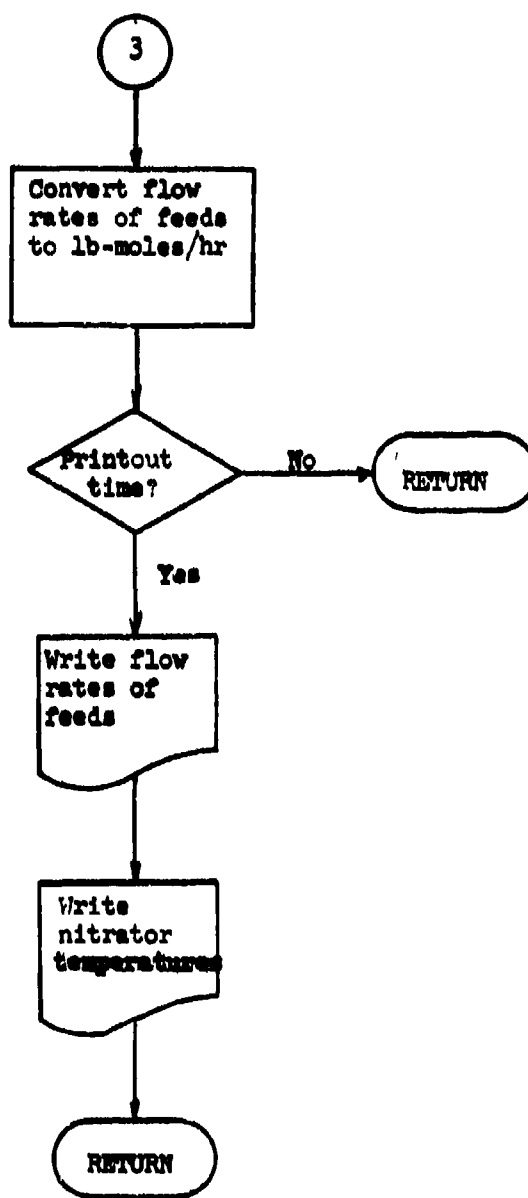


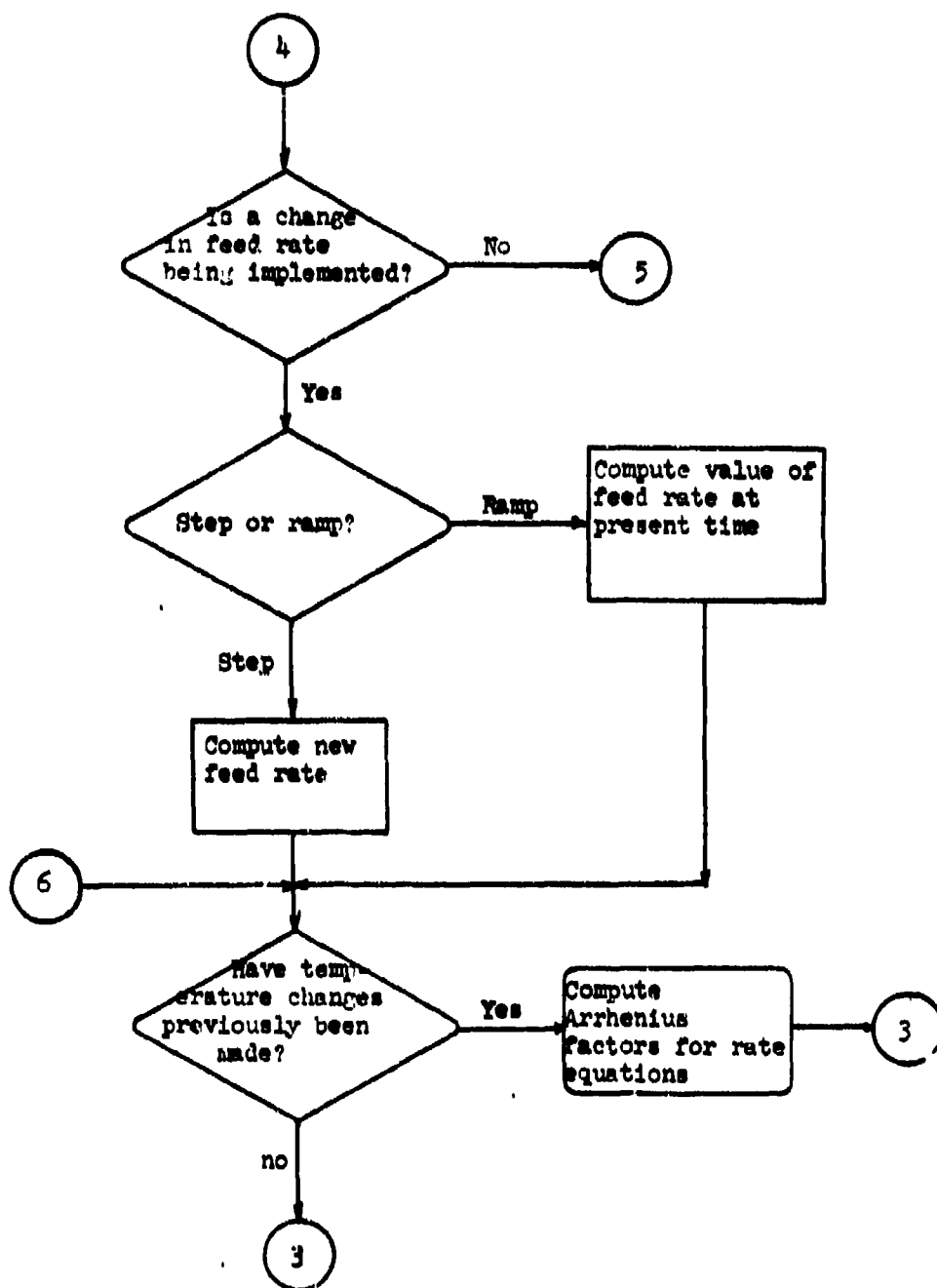
Subroutine INPT

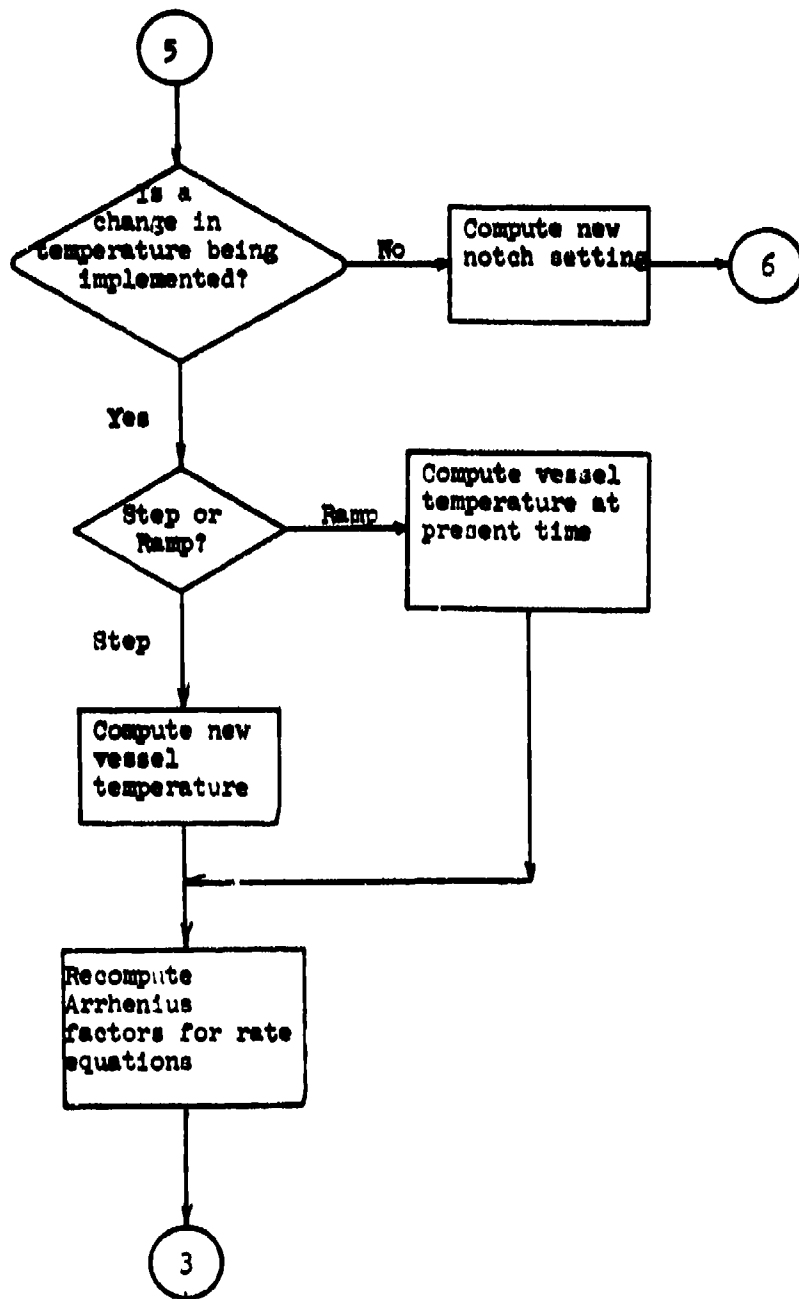




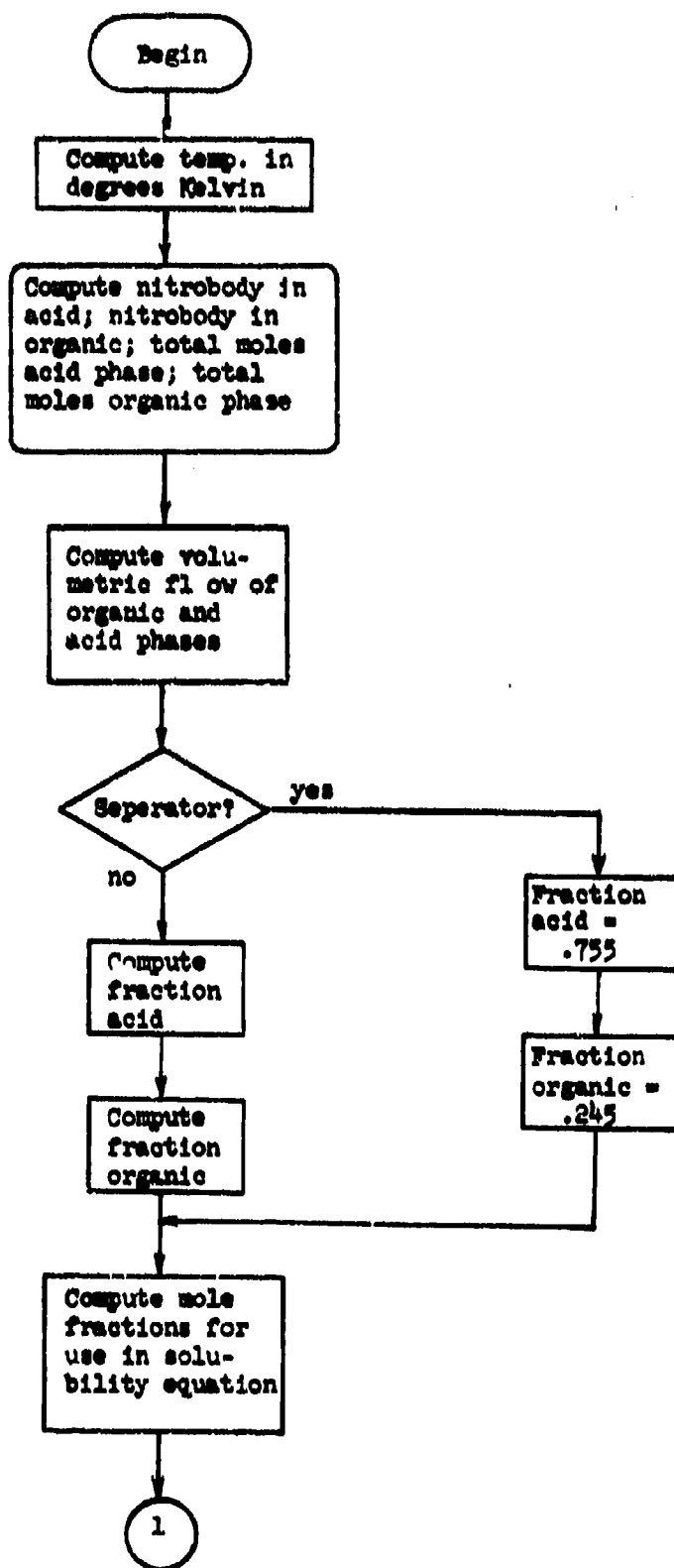


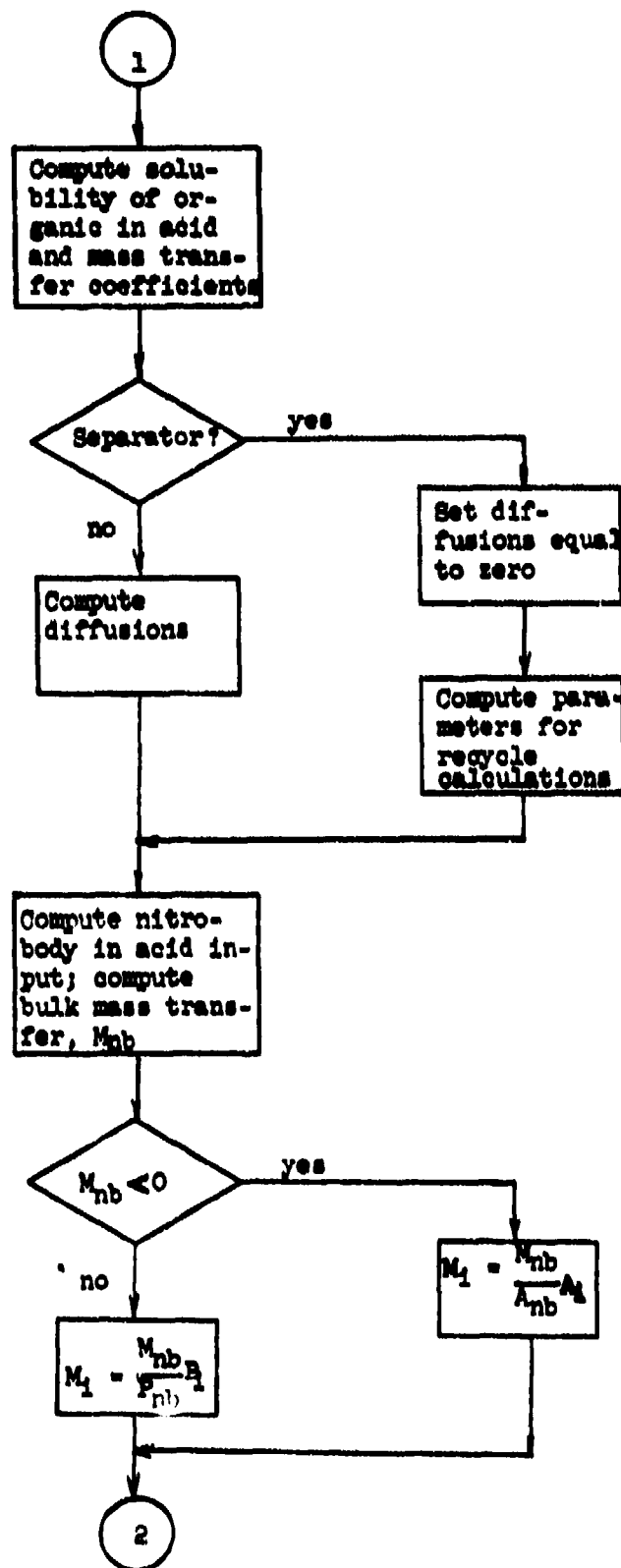


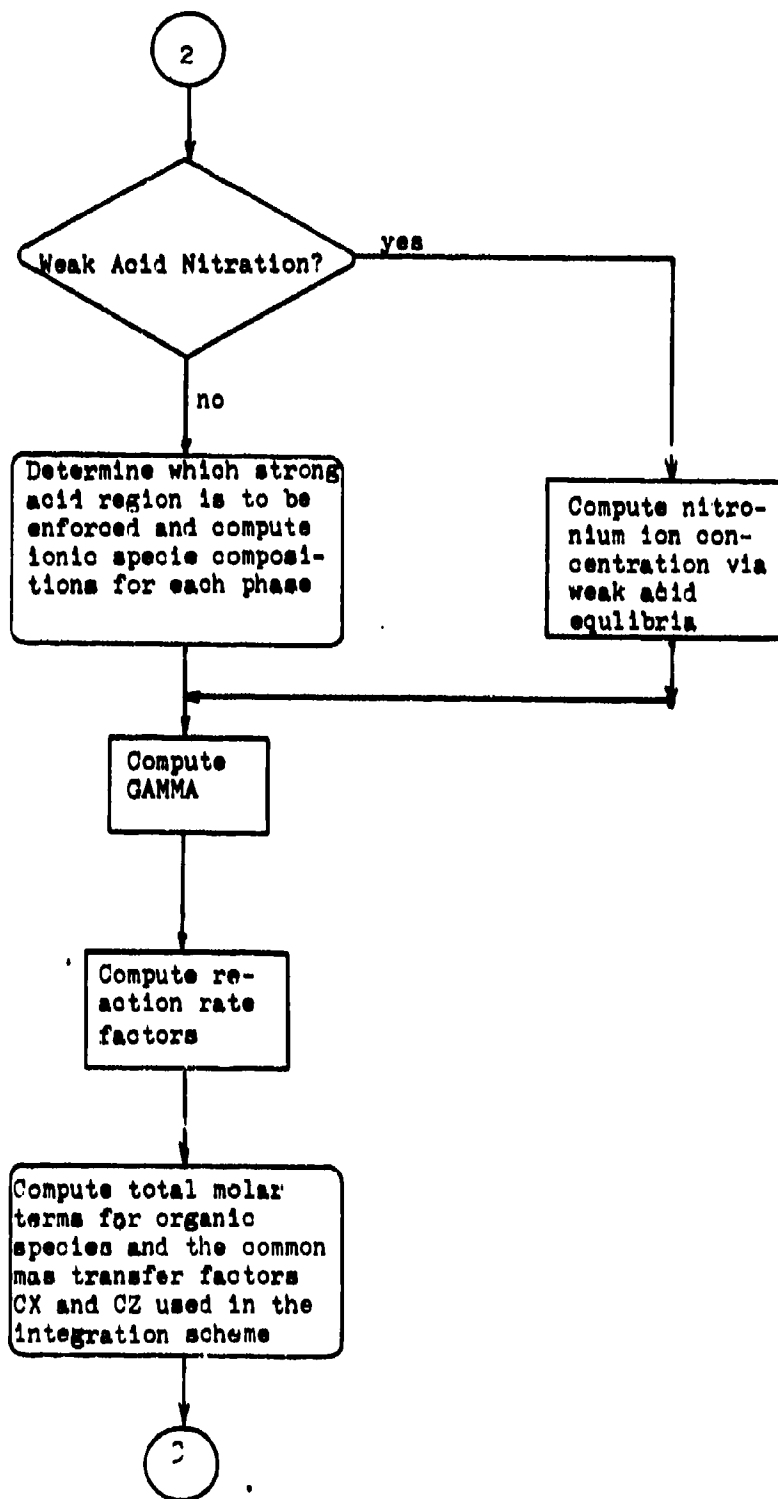


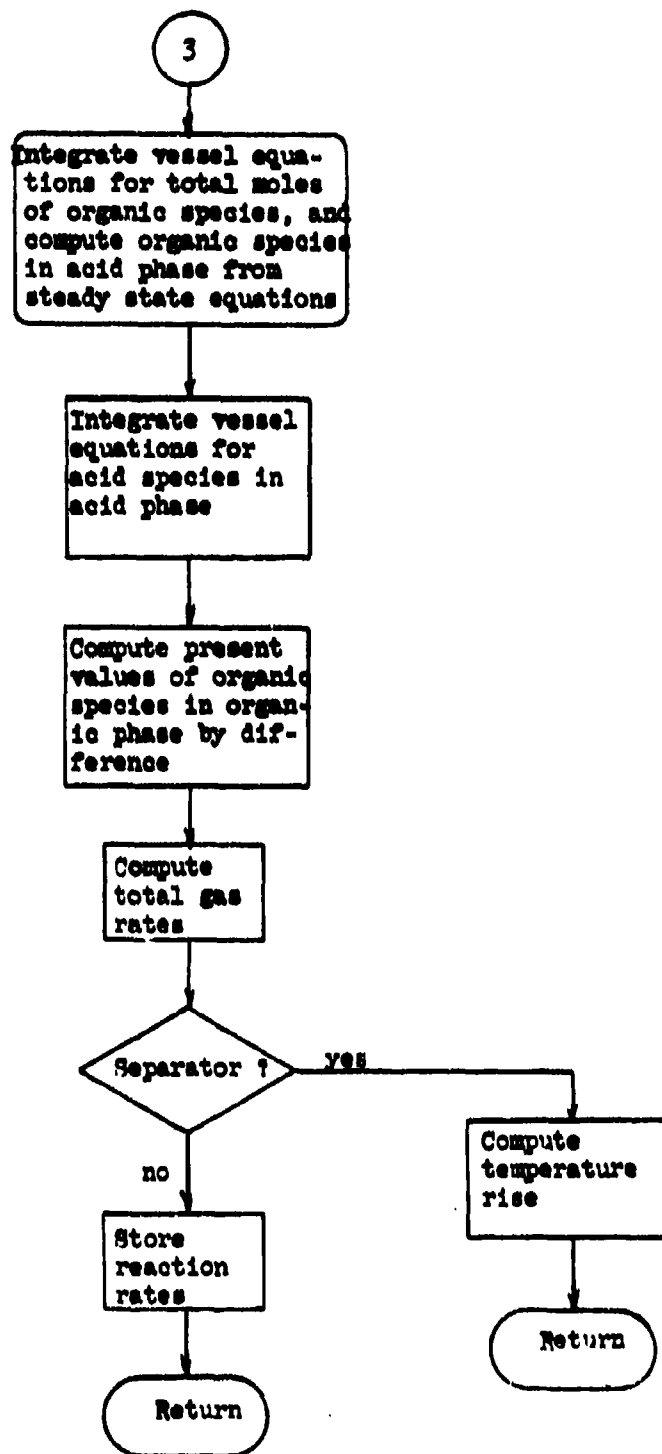


Subroutine SUB

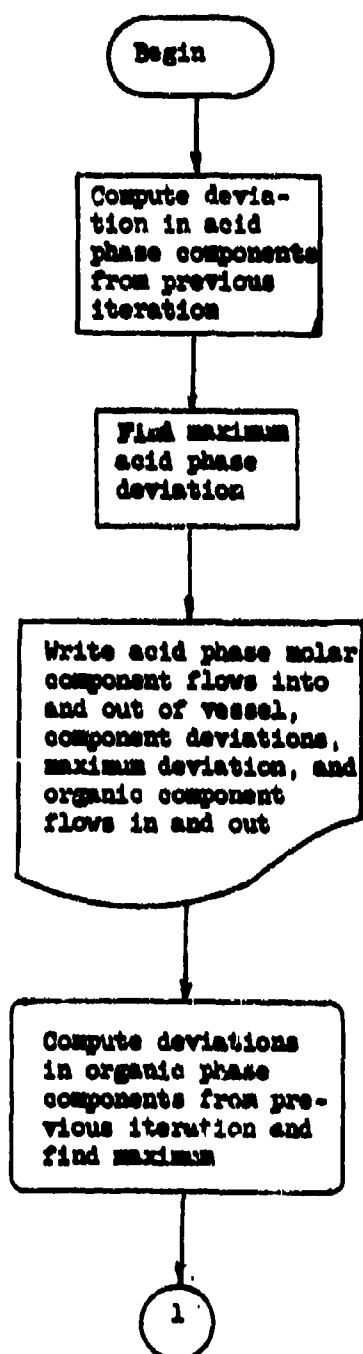


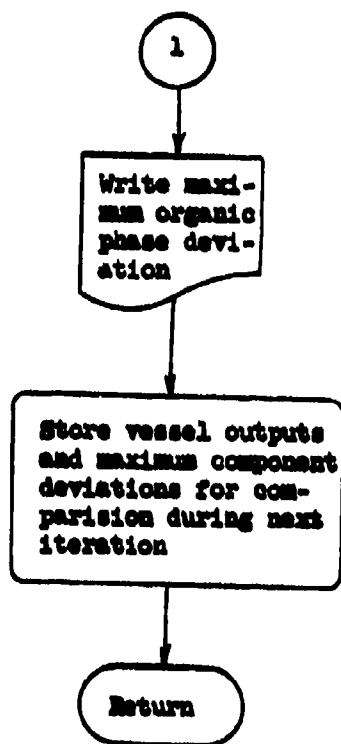




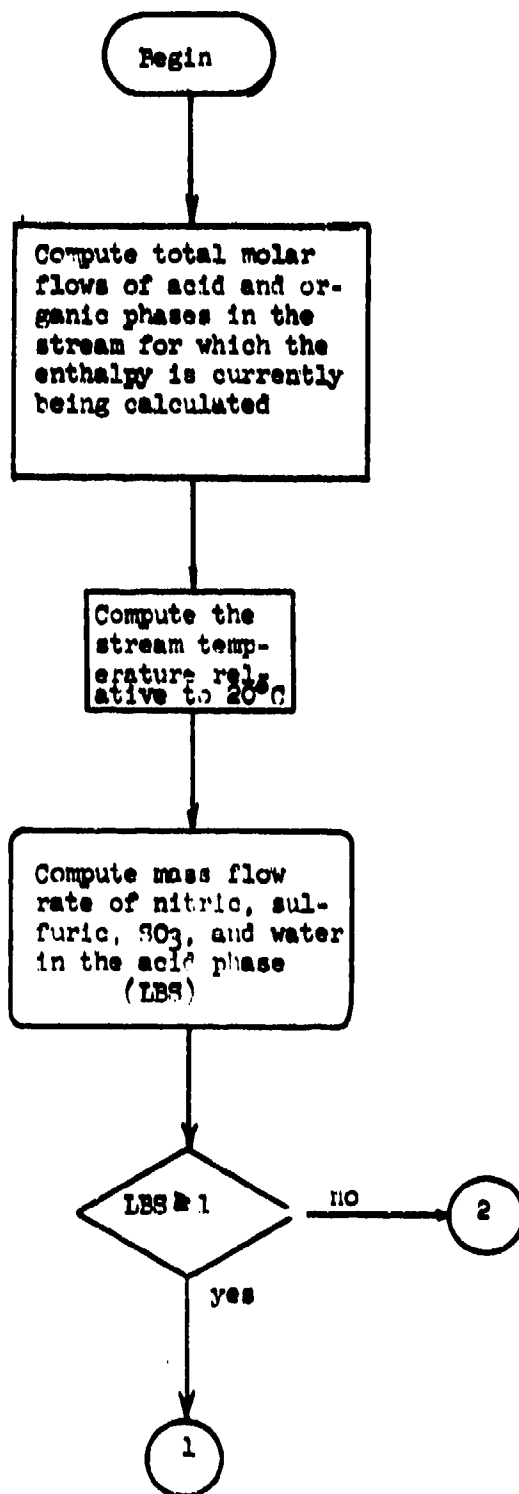


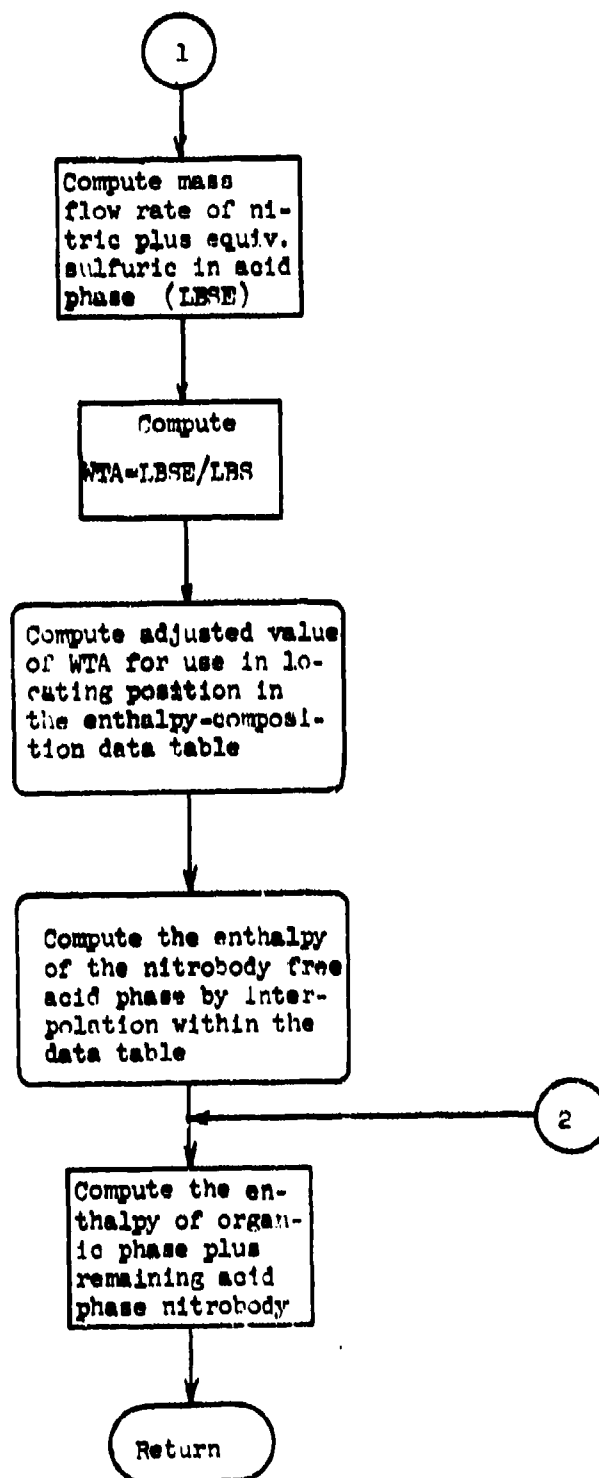
Subroutine SUB1





Function ENTH





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APPENDIX D

Dynamic Simulation--Program Nomenclature

Main Program

A (I)	moles/hr of component i in the total acid phase leaving the vessel currently being calculated
AA (I,J)	moles/hr of component i in the stream phase j of the separator currently being calculated
AF (I)	moles/hr of component i in the acid phase of the organic stream leaving a separator
AI (I)	moles/hr of component i in the total acid phase input to the vessel currently being calculated
AIR (I)	moles/hr of component i in the acid phase of the internal recycle leaving a separator
AKMA	acid phase mass transfer coefficient
AK10	rate constant for reaction 10
AK12	ratio of rate constants for reactions 1 and 2
AK3S	rate constant for reaction 3 in strong acid
AK3W	rate constant for reaction 3 in weak acid. NOT USED
AK4S	rate constant for reaction 4 in strong acid
AK4W	rate constant for reaction 4 in weak acid. NOT USED
AK5S	rate constant for reaction 5 in strong acid
AK6S	rate constant for reaction 6 in strong acid
AK7	rate constant for reaction 7
AK8	rate constant for reaction 8

AK9	NOT USED
AN(I,J)	percent actual nitric acid in the acid phase of the external recycle leaving separator j at the end of the i th plot interval
ANA(I,J)	amount of α - nitration taking place in nitrator j at the end of the i th plot interval
ANAC	running sum used in computation of ANA(I,J)
ANM(I,J)	amount of m-nitration taking place in nitrator j at the end of the i th plot interval
ANMC	running sum used in computation of ANM(I,J)
ANT(I,J)	moles/hr component i in the total acid phase leaving nitrator j
ARRAY(I,J)	moles/hr of component i from fresh acid feeds to nitrator j
AS(I,J)	moles/hr of component i in the total acid phase leaving separator j
ATM(I)	total moles/hr of stream phase i leaving the separator currently being calculated
ATW(I)	total lb/hr of stream phase i leaving the separator currently being calculated
AV(I,J)	initial value of moles/hr component j in the total acid phase leaving vessel i
AVL(I)	total cu ft/hr of stream phase i leaving the separator currently being calculated
AXR(I)	moles/hr of component i in the acid phase of the external recycle leaving a separator
A1A(I)	moles/hr of component i in the acid phase leaving nitrator 1A

A1AI (I)	moles/hr of component i in the fresh acid feeds to nitrator 1A
A1B (I)	moles/hr of component i in the acid phase leaving nitrator 1B
A1BI (I)	moles/hr of component i to nitrator 1B from fresh acid feeds
A1S (I)	moles/hr of component i in the total acid phase leaving separator 1
A2 (I)	moles/hr of component i in the acid phase leaving nitrator 2
A2I (I)	moles/hr of component i to nitrator 2 from fresh acid feeds
A2S (I)	moles/hr of component i in the total acid phase leaving separator 2
A3A (I)	moles/hr of component i in the acid phase leaving nitrator 3A
A3AI (I)	moles/hr of component i to nitrator 3A from fresh acid feeds
A3B (I)	moles/hr of component i in the acid phase leaving nitrator 3B
A3BI (I)	moles/hr of component i to nitrator 3B from fresh acid feeds
A3S (I)	moles/hr of component i in total acid phase leaving separator 3
A4 (I)	moles/hr of component i in acid phase leaving nitrator 4
A4S (I)	moles/hr of component i in total acid phase leaving separator 4
A4I (I)	moles/hr of component i to nitrator 4 from fresh acid feeds

A5(I)	moles/hr of component i in acid phase leaving nitrator 5
A5I(I)	moles/hr of component i to nitrator 5 from fresh acid feeds
A5S(I)	moles/hr of component i in the total acid phase leaving separator 5
A6(I)	moles/hr of component i in the acid phase leaving nitrator 6
A6I(I)	moles/hr of component i to nitrator 6 from fresh acid feeds
A6S(I)	moles/hr of component i in the total acid phase from separator 6
BASIS	NOT USED
CDNT	weight % DNT in crude TNT leaving separator 6
CDNTSA	weight % DNT in the nitrobody dissolved in the spent acid
CHAMXO	NOT USED
CHPMXO	NOT USED
CNBSA	weight % nitrobody dissolved in the acid phase of the spent acid leaving separator 1
CP(I)	specific heat of component i
CRUDE	lb/hr crude TNT leaving separator 6 (i.e., the mass flow of the total organic stream leaving separator 6)
CWSA	weight % water in the acid phase of the spent acid leaving separator 1

DENS (I,J)	specific gravity of the organic phase of any of the streams leaving the j th separator at the end of the i th plot interval
DENSA (I,J)	specific gravity of the acid phase in any of the streams leaving the j th separator at the end of the i th plot interval
DFAMXQ	maximum % change in an acid phase component between two successive iterations of the nitration section
DFPMXQ	maximum % change in an organic phase component between two successive iterations of the nitration section
DH (I)	heat of reaction for the i th reaction in BTU/lb-mole of reactant
DLT	estimated temperature of entrained organic phase that would be returned to nitrator 1B from the after separator
DT	integration time step (hrs)
DTPR	time between plotted points (mins)
EAQ (I)	molar ratio of acid phase in the organic stream to total organic stream leaving the i th separator
EAQP (I)	molar ratio of acid to organic phase in the organic stream leaving the i th separator
EAQP1	equivalent to EAOP (1)
EAQP2	equivalent to EAOP (2)
EAQP3	equivalent to EAOP (3)
EAQP4	equivalent to EAOP (4)
EAQP5	equivalent to EAOP (5)



EAQP6	equivalent to EAOP (6)
EAP	value of EAOP (I) for the separator currently being calculated
EFR	enthalpy of mixing for fume recovery acid
EQA (I)	molar ratio of organic phase in the external recycle to total external recycle leaving the separator i
EQAP (I)	molar ratio of organic to acid phase in either of the acid recycle streams leaving the ith separator
EQAP1	equivalent to EOAP (1)
EQAP2	equivalent to EOAP (2)
EQAP3	equivalent to EOAP (3)
EQAP4	equivalent to EOAP (4)
EQAP5	equivalent to EOAP (5)
EQAP6	equivalent to EOAP (6)
EQL	enthalpy of mixing for 40% oleum
EOP	value of EOAP (I) for the separator currently being calculated
EWN	enthalpy of mixing for weak nitric acid
EX	imposed upper bound on the Arrhenius coefficient in the reaction rate expressions for reactions 3 and 4 (MNT to DNT)
EYW	enthalpy of mixing for yellow water
E10	activation energy for reaction 10
E21	ratio of activation energies for reactions 2 and 1

E3S	activation energy for reaction 3 in a strong acid medium
E3W	NOT USED
E4S	activation energy for reaction 4 in a strong acid medium
E4W	NOT USED
E5S	activation energy for reaction 5 in a strong acid medium
E6S	activation energy for reaction 6 in a strong acid medium
E7	activation energy for reaction 7
E8	activation energy for reaction 8
E9	NOT USED
FA (I)	ratio of acid phase leaving 1 th separator that is recycled to total acid phase leaving the 1 th separator (fraction of acid phase recycled)
FACID (I)	ratio of acid phase leaving the 1 th separator in the organic stream forward to total acid phase leaving the 1 th separator (fraction of acid phase sent forward)
FACID1	equivalent to FACID (1)
FACID2	equivalent to FACID (2)
FACID3	equivalent to FACID (3)
FACID4	equivalent to FACID (4)
FACID5	equivalent to FACID (5)
FACID6	equivalent to FACID (6)

FAFR	fraction of total acid phase leaving separator 1 that appears in the external recycle from that separator
FAR	fraction of total acid phase leaving the separator that is recycled for the separator currently being calculated
FA1	equivalent to FA (1)
FA2	equivalent to FA (2)
FA3	equivalent to FA (3)
FA4	equivalent to FA (4)
FA5	equivalent to FA (5)
FA6	equivalent to FA (6)
FD	extent of reaction for nitrosylsulfuric decomposition
FIN(I,J)	lb/hr of feed i to nitration vessel j
FMAX	maximum allowable volumetric flow of internal acid recycle
FMX	equivalent to FMAX
FQ(I)	ratio of organic phase leaving the i th separator with the organic stream forward to total organic phase leaving the i th separator (fraction organic phase forward)
FORG(I)	ratio of organic phase leaving the i th separator with the acid recycle streams to total organic phase leaving the i th separator
FORG1	equivalent to FORG (1)

FORG2	equivalent to FORG (2)
FORG3	equivalent to FORG (3)
FORG4	equivalent to FORG (4)
FORG5	equivalent to FORG (5)
FORG6	equivalent to FORG (6)
FQ1	equivalent to FQ (1)
FQ2	equivalent to FQ (2)
FQ3	equivalent to FQ (3)
FQ4	equivalent to FQ (4)
FQ5	equivalent to FQ (5)
FQ6	equivalent to FQ (6)
FPQ	fraction of organic phase leaving a separator that appears in the organic stream forward for the separator currently being calculated
FR (I)	ratio of external recycle stream to total recycle leaving the i th separator
FRAC	ratio of internal recycle stream to total recycle leaving the separator currently being calculated
FRAC1	equivalent to FRC (1)
FRAC2	equivalent to FRC (2)
FRAC3	equivalent to FRC (3)
FRAC4	equivalent to FRC (4)
FRAC5	equivalent to FRC (5)

FRAC8	equivalent to FRC (8)
FRC (I)	ratio of internal recycle stream to total recycle stream leaving the <i>i</i> th separator
FR1	equivalent to FR (1)
FR2	equivalent to FR (2)
FR3	equivalent to FR (3)
FR4	equivalent to FR (4)
FR5	equivalent to FR (5)
FR6	equivalent to FR (6)
FV (I)	volume of the <i>i</i> th nitrator (cu ft)
FVKM	volume of the vessel currently being calculated
FVKMS	volume of a separator (all separators have the same volume)
FVKM1A	volume of nitrator 1A; equivalent to FV (1)
FVKM1B	volume of nitrator 1B; equivalent to FV (2)
FVKM2	volume of nitrator 2; equivalent to FV (3)
FVKM3A	volume of nitrator 3A; equivalent to FV (4)
FVKM3B	volume of nitrator 3B; equivalent to FV (5)
FVKM4	volume of nitrator 4; equivalent to FV (6)
FVKM5	volume of nitrator 5; equivalent to FV (7)
FVKM6	volume of nitrator 6; equivalent to FV (8)
G1 (I)	ratio of Arrhenius coefficients in the kinetic rate expressions for reaction 1 and 2 in the <i>i</i> th nitrator

G10 (I)	value of the Arrhenius coefficient in the kinetic rate expression for reaction 10 in the i^{th} nitrator
G3 (I)	NOT USED
G3S (I)	value of the Arrhenius coefficient in the kinetic rate expression for reaction 3 in the i^{th} nitrator under strong acid conditions
G4S (I)	NOT USED
G4S (I)	same as G3S (I) but for reaction 5
G5 (I)	value of Arrhenius coefficient in the kinetic rate expression for reaction 5 in the i^{th} nitrator
G6 (I)	same as G5 (I) but for reaction 6
G7 (I)	same as G5 (I) but for reaction 7
G8 (I)	same as G5 (I) but for reaction 8
G9 (I)	NOT USED
I	DO LOOP index
IC	counter for plotting intervals
ICALL	flag for first call to SUBROUTINE INPT
ICOUNT	equivalent to IC
IN	DO LOOP index for certain loops pertaining to nitrators
IPNCH	I/O device number for punched cards
IPRNT	print control flag: 0 summary printout only 1 debug printout of internal calculations during each integration step

IQUIT	number of stages being simulated
IS	DO LOOP index for certain loops pertaining to separators
ISTGE	stage number
ITYPE	vessel type flag: ITYPE=0 for nitrator ITYPE=1 for separator
IV	nitrating vessel number
IVSL	general vessel number
J	DO LOOP counter and generally used integer operator
JACK	counter for integration time steps
K	DO LOOP counter and generally used integer operator
MW(I)	molecular weight of component i
NM	integer number of integration passes through the process (or iterations) required for a particular run. Also the integer number of integration time steps required for the run
NN	integer number of iterations between summary printouts
NQ(I)	notch setting on internal recycle gate valve for separator i
NOTCH	notch setting for the separator currently being calculated
NP	integer number of iterations between computations of process performance indicators and other data for plotting

N1	equivalent to $NQ(1)$
N2	equivalent to $NQ(2)$
N3	equivalent to $NQ(3)$
N4	equivalent to $NQ(4)$
N5	equivalent to $NQ(5)$
N6	equivalent to $NQ(6)$
P(I)	moles/hr of component i in the total organic phase leaving the vessel currently being calculated
PA	lb/hr of total acid phase leaving a separator for which acid phase specific gravity is being calculated
PF(I)	moles/hr component i in the organic phase of the organic stream leaving a separator
PI(I)	moles/hr component i in the total organic phase input to the vessel currently being calculated
PIR(I)	moles/hr of component i in the organic phase of the internal recycle leaving a separator
PNT(I,J)	moles/hr of component i in the total organic phase leaving nitrator j
PP	lb/hr of total organic phase leaving a separator for which organic phase specific gravity is being calculated
PS(I,J)	moles/hr of component i in the total organic phase leaving the jth separator
PV(I,J)	initial value of moles/hr component j in the total organic phase leaving vessel i

U

PXR(I)	moles/hr of component i in the organic phase of the external recycle leaving a separator
P1A(I)	moles/hr of component i in the organic phase leaving nitrator 1A
P1AI(I)	moles/hr of component i in the organic feed stream to nitrator 1A (moles/hr toluene to 1A)
P1B(I)	moles/hr of component i in the organic phase leaving nitrator 1B
P1BI(I)	moles/hr of component i in the organic feed stream to nitrator 1B (moles/hr toluene to 1B)
P1S(I)	moles/hr component i in the total organic phase leaving separator 1
P2(I)	moles/hr component i in the organic phase leaving nitrator 2
P2S(I)	moles/hr component i in the total organic phase leaving separator 2
P3A(I)	moles/hr component i in the organic phase leaving nitrator 3A
P3B(I)	moles/hr component i in the organic phase leaving nitrator 3B
P3S(I)	moles/hr component i in the total organic phase leaving separator 3
P4(I)	moles/hr component i in the organic phase leaving nitrator 4
P4S(I)	moles/hr component i in the total organic phase leaving separator 4
P5(I)	moles/hr component i in the organic phase leaving nitrator 5

P5S (I)	moles/hr component i in the total organic phase leaving separator 5
P6 (I)	moles/hr component i in the organic phase leaving nitrator 6
P6S (I)	moles/hr component i in the total organic phase leaving separator 6
Q	accumulation term used in calculation of nitrator heat loads
QA	volumetric flow of total acid phase leaving a separator for which acid phase specific gravity is being calculated
QN (I,J)	heat load in nitrator j calculated at the end of the i th plotting interval
QP	volumetric flow of total organic phase leaving a separator for which organic phase specific gravity is being calculated
QY (I)	fraction of nitric acid converted to nitronium ions in nitration vessel i
R (I)	NOT USED
RATES (I,J)	rate of reaction j in nitration vessel i
RHQ (I)	molar density of component i
RHQ1	equivalent to RHQ (1)
RHQ10	equivalent to PHQ (10)
RHQ11	equivalent to RHQ (11)
RHQ12	equivalent to RHQ (12)
RHQ13	equivalent to RHQ (13)
RHQ14	equivalent to RHQ (14)

Q

RHQ2	equivalent to RHQ (2)
RHQ3	equivalent to RHQ (3)
RHQ4	equivalent to RHQ (4)
RHQ5	equivalent to RHQ5
RHQ6	equivalent to RHQ (6)
RHQ7	equivalent to RHQ (7)
RHQ8	equivalent to RHQ (8)
RHQ9	equivalent to RHQ (9)
RNS (I,J)	nitric to sulfuric acid ratio in nitration vessel j calculated at the end of the i th plotting interval (for acid phase only)
RNSS (I,J)	nitric to sulfuric acid ratio in separator j calculated at the end of the i th plotting interval (for acid phase only)
RP	coefficient on the molecular oxygen term in reaction 9
RR	ideal gas law constant
SA	adjustable constant. NOT USED
SB	equivalent to organic phase mass transfer coefficient (KMAP)
SC	equivalent to AKEQ4 in SUBROUTINE SUB
SD	NOT USED
SE	equivalent to AK9. NOT USED
SG	equivalent to E9. NOT USED

SH	equivalent to AKEQ1 in SUBROUTINE SUB
SI	NOT USED
SJ	equivalent to AKEQ3 in SUBROUTINE SUB
SPA	accumulator term used in calculation of spent acid mass flow rate
SPENT (I)	spent acid mass flow rate at the end of the i th plotting interval (flow rate of acid phase of the external recycle stream leaving separator 1)
SPQ	mass flow rate of dissolved organic in the spent acid
SUM	accumulator term used in calculation of the mass flow rate of crude TNT leaving separator 8
T	temperature of nitration vessel currently being calculated
TDNT	mass flow rate of DNT in the total organic stream leaving separator 8
TCOX	cumulative total moles/hr oxides of carbon (gas) leaving all vessels in the nitration section during a given iteration
TEMP (I)	temperature of the i th nitration vessel
TI	NOT USED
TIME	simulated elapsed time since beginning of run
TLBS	total lb/hr of acid phase leaving a separator on a nitrobody free basis. Used in computation of acid concentration indicators
TM (I)	total moles/hr of stream i leaving a separator currently being calculated

TNOX	total moles/hr oxides of nitrogen (gas) leaving all vessels in the nitration section during a given iteration
TR	reference temperature
TSEP (I)	computed temperature of the separator currently being calculated
TTCOX (I)	same as TCOX except that value is particular value at the end of the i^{th} plotting interval
TTME	total time of process operation to be simulated
TTNOX (I)	same as TNOX except that value is particular value at the end of the i^{th} plotting interval
TVL (I)	volumetric flow (cu ft/hr) of the i^{th} stream leaving the separator currently being calculated
TW (I)	mass flow (lb/hr) of the i^{th} stream leaving the separator currently being calculated
T1A	temperature of nitrator 1A (equivalent to TEMP (1))
T1B	temperature of nitrator 1B (equivalent to TEMP (2))
T2	temperature of nitrator 2 (equivalent to TEMP (3))
T3A	temperature of nitrator 3A (equivalent to TEMP (4))
T3B	temperature of nitrator 3B (equivalent to TEMP (5))
T4	temperature of nitrator 4 (equivalent to TEMP (6))
T5	temperature of nitrator 5 (equivalent to TEMP (7))
T6	temperature of nitrator 6 (equivalent to TEMP (8))
VKM (I)	volume of the i^{th} nitrator
VKMS	volume of a separator (same for all separators)

X(I) elapsed simulated time at the end of the *i*th plotting interval (nomenclature is specific to plotting routine for plotting one dimensional variables as a function of time)

XX(I,J) elapsed simulated time at the end of the *i*th plotting interval (this form of elapsed time is used for plotting variables of up to *j* dimension)

XXX(I) moles/hr nitric acid in the acid phase converted to nitronium ions in nitration vessel *i*

Subroutine INPT

The definitions of the following variables are identical to those in the main program: AF(I), AIR(I), AKMA, AKMATL, AK10, AK12, AK3S, AK3W, AK4S, AK4W, AK5S, AK6S, AK7, AK8, AK9, ARRAY(I,J), AXR(I), A1S(I), A2S(I), A3S(I), A4S(I), A5S(I), A6S(I), CP(I), DH(I), DT, EAQP1, EAQP2, EAQP, EAQP3, EAQP4, EAQP5, EAQP6, EQAP1, EQAP2, EQAP3, EQAP4, EQAP5, EQAP6, EX, E10, E21, E3S, E3W, E4S, E4W, E5S, E6S, E7, E8, E9, FAC1D1, FAC1D2, FAC1D3, FAC1D4, FAC1D5, FAC1D6, FA1, FA2, FA3, FA4, FA5, FA6, FIN(I,J), FMX, FORG1, FORG2, FORG3, FORG4, FORG5, FORG6, FQ1, FQ2, FQ3, FQ4, FQ5, FQ6, FRAC1, FRAC2, FRAC3, FRAC4, FRAC5, FRAC6, FR1, FR2, FR3, FR4, FR5, FR6, FVKM1A, FVKM1B, FVKM2, FVKM3A, FVKM3B, FVKM4, FVKM5, FVKM6, G1(I), G10(I), G3(I), G3S(I), G4(I), G4S(I), G5(I), G6(I), G7(I), G8(I), G9(I), ICALL, IPRT, JACK, MW(I), NM, NN, NP, N1, N2, N3, N4, N5, N6, PF(I), PIR(I), PXR(I), P1AI(I), P1BI(I), P1S(I), P2S(I), P3S(I), P4S(I), P5S(I), P6S(I), RATES(I,J), RHQ1, RHQ10, RHQ11, RHQ12, RHQ13, RHQ14, RHQ2, RHQ3, RHQ4, RHQ5, RHQ6, RHQ7, RHQ8, RHQ9, RP, RR, SA, SB, SC, SD, SE, SG, SH, SI, SJ, TCOX, TEMP(I), TNOX, TR, TSEP(I), TTME, T1A, T1B, T2, T3, T4, T5, T6,

Remaining variables are defined as follows:

COMP(I,J) weight % component *i* in feedstock type *j*

DDL fractional part of a change in feed rate or nitrator temperature which is applied to the process during a given iteration

DL(I) magnitude of the *i*th change in an independent variable

ICH (J)	integer code number for the independent variable type to which the j th change is being made
IKT	flag to indicate whether or not temperature changes have been made to the initial conditions
IPRNT	simulated time between summary printouts
IVS (J)	integer code number for the vessel to which the j th change in one of the independent variable types is made
NCHNG	number of given change which is to be made during the run
NOTCH (I)	notch setting on internal recycle gate value for the i th separator
NTME (I)	number of iterations between the beginning of a run the initiation of the i th change in an independent variable
NTVL (I)	number of iterations over which the magnitude of the i th change is to be equally distributed (used for ramping an independent variable)
TME	simulated time at which a given change is to be initiated
TVL	simulated time interval over which a given change is to be made
ZA	temperature coefficient in the exponent of the Arrhenius rate expression

Subroutine SUB

The definitions of the following variables are identical to those in the main program: A(I), AI(I), AKMA, AKMATL, AK10, AK12, AK3S, AK3W, AK4S, AK4W, AK5S, AK6S, AK7, AK8, CP(I), DH(I), DT, EX, E10, E21, E3W, E3S, E4W, E4S, E6S, E7, E8, FAlI, FD, FMX, FPQ, E5S, FRAC, FVKM, G1(I), G10(I), G3(I), G3S(I), G4(I), G4S(I), G5(I), G3(I), G7(I), G8(I), G9(I), ICALL, IFRNT, ISTGE, ITYPE, IV, JACK, NM, NN, NOTCH, NP, P(I), PI(I), QY(I), RATES(I,J), RHQ1, RHQ11, RHQ12, RHQ13, RHQ14, RHQ2, RHQ3, RHQ4, RHQ5, RHQ6, RHQ7, RHQ8, RHQ9, RR, RP, SA, SB, SC, SD, SE, SG, SH, SI, SJ, T, TCOX, TI, TNOX, TR, TSEP(I), TTME, XYY(I)

The definitions of the following variables are identical to other variables defined for the main program:

<u>Variable in SUB</u>	<u>Variable in main program</u>
AI1 thru AI17	AI (1) thru AI (17)
A1 thru A17	A (1) thru A (17)
EAQP	EAP
EQAP	EQP
PI1 thru PI17	PI (1) thru PI (17)
P1 thru P17	P (1) thru P (17)

Remaining variables are defined as follows:

AINB	moles/hr nitrobody in the aggregate acid phase input to the vessel currently being calculated
AKA	general rate factor for all nitration reactions. Also if Bennett's strong acid rate expression is used, the coefficient of the besulfate ion concentration
AKB	coefficient of the sulfuric acid concentration in Bennett's rate expression
AKC	coefficient of the pyrosulfate ion concentration in Bennett's rate expression



AKEQ	equilibrium constant for the dissociation of sulfuric acid in an aqueous medium
AKEQOV	equilibrium constant for the dissociation of a mixture of sulfuric and pyrosulfuric acids to ionic species. NOT USED
AKEQ1	equilibrium constant for the dissociation of nitric acid in aqueous sulfuric acid
AKEQ2	equivalent to AKEQ
AKEQ3	equilibrium constant for the dissociation of nitric acid in anhydrous sulfuric acid
AKEQ4	equilibrium constant for the recombination of nitronium and bisulfate ions in anhydrous acid mixtures
AKMAP	organic phase mass transfer coefficient
AK1	computed value of AKEQ1 obtained from interval halving procedure
AK3	computed value of AKEQ3 obtained from interval halving procedure
AK4	computed value of AKEQ4 obtained from interval halving procedure
AL	moles/hr water in the total acid phase of the vessel current being calculated; can have negative value which then represents moles/hr SO_2
AMNB	moles/hr nitrobody transferred from organic to acid phase by bulk mass transfer; negative value means transfer from acid to organic phase
AM1	moles/hr μMNT transferred by bulk mass transfer
AM2	same as AM1 but for mMNT

AM3	same as AM1 but for cDNT
AM4	same as AM1 but for mDNT
AM5	same as AM1 but for cTNT
AM6	same as AM1 but for mTNT
AM7	same as AM1 but for TNE
AM8	same as AM1 but for TNBX
ANB	total moles/hr of nitrobody dissolved in the acid phase leaving the vessel currently being calculated
ASO4	combined moles/hr of SO_2 and H_2SO_4 in the acid phase leaving the vessel currently being calculated
AT	total moles/hr of acid phase leaving the vessel currently being calculated
A11QA	concentration (moles/ft ³) of sulfuric acid in the acid phase of the vessel currently being calculated
B	initial concentration (moles/ft ³) of free sulfuric acid in the acid phase of the vessel currently being calculated
BC	$3 + (3 \times C)$
C	initial concentration (moles/ft ³) of pyrosulfuric acid in the acid phase of the vessel currently being calculated
CB	$(.5 \times B) + (1.5 \times C)$
CF	C-F
CHNO3	equilibrium concentration of nitric acid in the acid phase of the vessel currently being calculated

CHSO4	equilibrium concentration of bisulfate ions in the acid phase of the vessel currently being calculated
CHSO7	equilibrium concentration of pyrosulfate ions in the acid phase of the vessel currently being calculated
CH2O	same as CHNO3 but for water
CH2SO4	equilibrium concentration of sulfuric acid in the acid phase of the vessel currently being calculated
CH3O	equilibrium concentration of hydronium ions in the acid phase of the vessel currently being calculated
CNO2	equilibrium concentration of nitronium ions in the acid phase of the vessel currently being calculated
CX	consolidation term for (ZA + YP)
CZ	consolidation term for (ZB - YA + 1 + CX)
C5	moles/hr nitrosylsulfuric acid produced by oxidation reactions in the vessel currently being calculated
CP5	moles/hr nitrosylsulfuric acid which remain undecomposed in the vessel currently being calculated
D	initial acid phase concentration of combined sulfuric acid plus pyrosulfuric acid in the vessel currently being calculated
DAL	rate of change of AL with respect to time in the vessel currently being calculated
DASO4	rate of change of ASO4 with respect to time in the vessel currently being calculated
DA1	rate of change of A1 with respect to time in the vessel currently being calculated

DA12	rate of change of A12 with respect to time in the vessel currently being calculated
DA2	rate of change of A2 with respect to time in vessel currently being calculated
DA3	rate of change of A3 with respect to time in the vessel currently being calculated
DA4	same as DA3 but for A4
DA5	same as DA3 but for A5
DA6	same as DA3 but for A6
DA7	same as DA3 but for A7
DA8	same as DA3 but for A8
DA9	same as DA3 but for A9
DELTA	acid concentration term in the weak acid nitration rate expression . NOT USED
DP1	rate of change of P1 with respect to time in the vessel currently being calculated
DP10	same as DP1 but for P10
DP2	same as DP1 but for P2
DP3	same as DP1 but for P3
DP4	same as DP1 but for P4
DP5	same as DP1 but for P5
DP6	same as DP1 but for P6
DP7	same as DP1 but for P7
DP8	same as DP1 but for P8



DTA	acid phase adjusted integration time step
DTP	organic phase adjusted integration time step
D1	moles/hr of α -MNT that diffuse into the acid phase in the vessel currently being calculated
D10	moles/hr of toluene which diffuse from the bulk organic phase to the acid-organic interface
D2	same as D1 but for m-MNT
D3	same as D1 but for α -DNT
D4	same as D1 but for m-DNT
D5	same as D1 but for α -TNT
D6	same as D1 but for m-TNT
D7	same as D1 but for TNB
D8	same as D1 but for TNBX
ETA	overall mass transfer coefficient in the vessel currently being calculated
ETAA	acid phase mass transfer coefficient in the vessel currently being calculated
ETAP	organic phase mass transfer coefficient in the vessel currently being calculated
ETATL	mass transfer coefficient for toluene
F	initial acid phase concentration of nitric acid in the vessel currently being calculated
FA	volumetric fraction of acid phase in the vessel currently being calculated



FF (I)	cross sectional area fraction corresponding to the ith notch setting on the gate valve in the internal recycle line of the separator currently being calculated
FOV	constant set equal to one
FP	volumetric fraction of organic phase in the vessel currently being calculated
F10A	reaction rate factor for reaction 10 where α -TNT is the reactant for the vessel currently being calculated
F10M	same as F10A but for m-TNT
F3	reaction rate factor for reaction 3 in the vessel currently being calculated
F4	same as F3 but for reaction 4
F5	same as F3 but for reaction 5
F6	same as F3 but for reaction 6
F7A	reaction rate factor for reaction 7 in the vessel currently being calculated where α -DNT is the reactant
F7M	same as F7A but for m-DNT
F8A	reaction rate factor for reaction 8 in the vessel currently being calculated where α -DNT is the reactant
F8M	same as F8A but for m-DNT
F9A	Zero
F9M	Zero

GAMMA	acid concentration term used in all nitration rate expressions
KLM	flag to indicate which nitration region exists in the vessel being calculated
PNB	total flow (moles/hr) of organic phase nitrobody components leaving the vessel currently being calculated
PP	exponent of nitrobody-in-acid- solubility correlation
Q	fraction nitric acid converted to nitronium ions for the vessel currently being calculated
QA	volumetric flow of the acid phase leaving the vessel currently being calculated
QP	volumetric flow of the organic phase leaving the vessel currently being calculated
QT	total volumetric flow of combined internal and external recycle leaving the separator currently being calculated
RATE (I)	rate of the i^{th} reaction in the vessel currently being calculated
R1	rate of reaction 1 in the vessel currently being calculated; equivalent to RATE(1) (moles/hr)
R10	same as R1 but for reaction 10; equivalent to RATE(10); also $R10A + R10M$
R10A	rate of reaction 10 in the vessel currently being calculated where α -TNT is the reactant
R10M	same as R10A but for m -TNT
R2	same as R1 but for reaction 2; equivalent to RATE(2)

R3	same as R1 but for reaction 3; equivalent to RATE (3)
R4	same as R1 but for reaction 4; equivalent to RATE (4)
R5	same as R1 but for reaction 5; equivalent to RATE (5)
R6	same as R1 but for reaction 6; equivalent to RATE (6)
R7	same as R1 but for the combined reaction 7; equivalent to RATE (7); also R7A + R7M
R7A	rate of reaction 7 in the vessel currently being calculated where α -DNT is the reactant
R7M	same as R7A but for m-DNT
R8	same as R1 but for the combined reaction 8; equivalent to RATE (8); also R8A + R8M
R8A	same as R7A but for reaction 8
R8M	same as R8A but for m-DNT
R9	same as R1 but for reaction 9; equivalent to RATE (9)
R9A	Zero
R9G	Zero
R9M	Zero
TKEL	temperature of the vessel currently being calculated ($^{\circ}$ K)
T1	A1 + P1
T2	A2 + P2



T3	A3 + P3
T4	A4 + P4
T5	A5 + P5
T6	A6 + P6
T7	A7 + P7
T8	A8 + P8
W	initial acid phase concentration of water in the vessel currently being calculated (moles/ft ³)
X	consolidation term used in the integration sequence of organic species in the acid phase of the vessel currently being calculated
XEQA	equilibrium solubility of nitrobody in the acid phase of the vessel currently being calculated (moles/hr)
XL	lower limit of an ionic species concentration which is applied during internal halving procedure
XU	upper limit of an ionic species concentration which is applied during internal halving procedure
XUP	upper limit of HS ₂ O ₇ concentration (resulting from dissociation according to equation 19) which is applied during internal halving procedure
X1	mole fraction α -MNT in the acid phase of the vessel currently being calculated
X13	mole fraction water in acid phase of the vessel currently being calculated
X14	mole fraction sulfur trioxide in the acid phase of the vessel currently being calculated

X2	mole fraction m-MNT in the acid phase of the vessel currently being calculated
X5	mole fraction α -TNT in the acid phase of the vessel currently being calculated
X6	mole fraction m-TNT in the acid phase of the vessel currently being calculated
X9	mole fraction nitric acid in the acid phase of the vessel currently being calculated
Y	consolidation term used in the integration sequence for organic species in the acid phase of the vessel currently being calculated; also used for initial concentration (moles/ft ³) of free sulfuric in the acid phase of the vessel currently being calculated
YA	ratio of AMNB to ANB
YP	ratio of AMNB to PNB
Z	initial acid phase concentration of nitric acid which is used under strong acid nitrating conditions for which water is present; also used as a consolidation term in the integration sequence for organic species in the acid phase
ZA	enthalpy of the contents of a separator (BTU/hr - °C)
ZB	rate of heat generated in a separator due to reaction (BTU/Hr)
ZD	A8-A17; undissociated acid phase nitric acid remaining at equilibrium in the vessel currently being calculated (moles/hr)

Subroutine SUB2

The definitions of the following variables are identical to those in the main program: AKMA, AKMATL, AK10, AK12, AK3S, AK3W, AK4S, AK4W, AK5S, AK6S, AK7, AK8, CP(I), DH(I), E10, E21, E3S, E3W, E4S, E4W, E5S, E6S, E7, E8, FD, DMX, QA, QP, RHO(I), RP, RR, SA, SB, SC, SD, SE, SG, SH, SI, SJ, TR

Remaining variables are defined as follows:

AQ(I)	moles/hr component i in the total acid phase leaving the separator for which recycle parameters are currently being calculated
AT	total moles/hr of acid phase leaving the separator for which recycle parameters are currently being calculated
EAQP	molar ratio of acid to organic phase in the organic stream leaving the separator for which recycle parameters are currently being calculated
EQAP	molar ratio of organic to acid phase in either of the recycle streams leaving the separator for which recycle parameters are currently being calculated
FAR	fraction of acid phase that is recycled in the separator for which recycle parameters are currently being calculated
FAR1	fraction of acid phase sent forward from the separator for which recycle parameters are currently being calculated
FF(I)	identical to definitions given in subroutine SUB
FFO	fraction of organic phase sent forward from the separator for which recycle parameters are currently being calculated

FPQ1 fraction of organic phase which is recycled in the separator for which recycle parameters are currently being calculated

FRAC ratio of internal recycle stream to total recycle streams leaving the separator for which recycle parameters are currently being calculated

NOTCH notch setting on the internal recycle gate valve for the separator for which recycle parameters are being calculated

PQ moles/hr component i the total organic phase leaving the separator for which recycle parameters are currently being calculated

PT moles/hr total organic phase leaving the separator for which recycle parameters are currently being calculated

QT volumetric flow (ft^3/hr) of combined recycle streams leaving the separator for which recycle parameters are currently being calculated

Subroutine SUB1

The definitions of the following variables are identical to those in the main program: AI(J), AKMA, AKMATL, AK10, AK12, AK3S, AK3W, AK4S, AK4W, AK5S, AK6S, AK7, AK8, AV(I,J), CHAMXQ, CP(I), DFAMXQ, DH(I), DT, EX, E10, E21, E3S, E3W, E4S, E4W, E5S, E6S, E7, E8, FD, FMX, G1(I), G10(I), G3(I), G3S(I), G4(I), G4S(I), G5(I), G6(I), G7(I), G8(I), G9(I), ICALL, IPRNT, IVSL, JACK, NM, NN, NP, PI(I), PV(I,J), QY(I), RATES(I,J), RHQ1, RHQ10, RHQ11, RHQ12, RHQ13, RHQ14, RHQ2, RHQ3, RHQ4, RHQ5, RHQ6, RHQ7, RHQ8, RHQ9, RP, RR, SA, SB, SC, SD, SE, SG, SH, SI, SJ, TCOX, TNOX, TR, TSEP(I), TTME, XYY(I)

Remaining variables are defined as follows:

AQ(I) moles/hr component i in the acid phase of the vessel for which component % changes are currently being calculated

DFA (I)	acid phase component i % change during NN iterations in the vessel currently being calculated
DFAMX	maximum % change in an acid phase component in the vessel currently being calculated
DFP (I)	same as DFA (I) but for organic phase
DFPMX	same as DFAMX but for organic phase
PQ (I)	moles/hr component i in the organic phase of the vessel for which component % changes are currently being calculated
R1-R10	NOT USED

Function ENTH

The definitions of the following variables are identical to those in the main program: AKMA, AKMATL, AK10, AK3S, AK3W, AK4S, AK4W, AK5S, AK6S, AK7, AK8, CP (I), DH (I), E10, E12, E3S, E3W, E4S, E4W, E5S, E6S, E7, E8, FD, FMAX, RHQ1, RHQ10, RHQ11, RHQ12, RHQ13, RHQ14, RHQ2, RHQ3, RHQ4, RHQ5, RHQ6, RHQ7, RHQ8, RHQ9, RR, SA, SB, SC, SD, SE, SG, SH, SI, SJ, TR

Remaining variables are defined as follows:

A (I)	moles/hr component i in the acid phase of the stream for which the enthalpy is currently being calculated
AX (I)	moles/hr component i in the total acid phase leaving a vessel for which the enthalpy of a particular leaving stream is currently being calculated
CP11	equivalent to CP (11)
CP12	equivalent to CP (12)
CP13	equivalent to CP (13)
CP14	equivalent to CP (14)

DLT	temperature of the vessel (relative to 20°C) for which the enthalpy of a particular exiting stream is currently being calculated
ENTH	enthalpy of the stream currently being calculated (kcal/hr)
ENTH0	enthalpy of mixing of the acid components in the acid phase of the stream currently being calculated based on the zero nitric curve of the McKinley and Brown data (kcal/lb)
ENTH2	enthalpy of mixing of the acid components in the acid phase of the stream currently being calculated based on the 20% nitric curve of the McKinley and Brown data (kcal/lb)
F	adjusted weight fraction of nitric acid plus sulfuric acid in the acid phase of the stream currently being calculated on a nitrobody free basis
LBS	lb/hr of nitric acid, sulfuric acid, water (or sulfur trioxide) in the acid phase of the stream currently being calculated
LBSE	lb/hr of nitric acid and equivalent sulfuric acid in the acid phase of the stream currently being calculated
P(I)	moles/hr component i in the organic phase of the stream for which the enthalpy is currently being calculated
PX(I)	moles/hr component i in the total organic phase leaving a vessel for which the enthalpy of a particular leaving stream is currently being calculated
T	moles/hr combined organic and acid phase nitro- body component in the stream for which enthalpy is currently being calculated

1

TP	temperature of the vessel for which the enthalpy of an exiting stream is being calculated (°C)
WTA	LBSE/LBS; nitrobody free weight fraction of equivalent sulfuric plus nitric acid in the acid phase of the stream for which the enthalpy is currently being calculated
WTN	weight fraction of nitric acid in the equivalent sulfuric plus nitric acid of the acid phase of the stream for which the enthalpy is currently being calculated
X(I)	the <i>i</i> th data point on the zero % nitric curve from the enthalpy concentration data of McKinley and Brown
XA1	FACID, FA or 1 dependent on the origination point of the stream for which the enthalpy is currently being calculated
XA2	FR, FRAC or 1 dependent on the origination point of the stream for which the enthalpy is currently being calculated
XP1	FØ, FØRG or 1 dependent on the origination point of the stream for which the enthalpy is currently being calculated
XP2	FR, FRAC or 1 dependent on the origination point of the stream for which the enthalpy is currently being calculated
Y(I)	the <i>i</i> th data point on the 20% nitric curve from the enthalpy concentration data of McKinley and Brown

APPENDIX E

Dynamic Simulation--Input Data Format

<u>Card</u>	<u>Data Read</u>	<u>Format</u>
1	AK12, AK3W, AK4W, AK5S, AK65, AK7, AK8, AK10	8F10.0
2	AK3S, AK47, E33, E4S	8F10.0
3	E21, E3W, E4W, E5S, E6S, E7, E8, E10	8F10.0
4	9A, 9B, 9C, 9D, 9E, 9G, 9H, 9I	8F10.0
5	9S, 9R, 9T, AKMA, AKMATL, FD, RP	8F10.0
6, 7	DH (I), I=1, 10	8F10.0
8, 9	RHY (I), I=1, 10	8F10.0
10, 11	CP (I), I=1, 14	8F10.0
12 - 14	A1A (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
14 - 16	P1A (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
17 - 19	A1B (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
20 - 22	P1B (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
23 - 25	A1S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
26 - 28	P1S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
29 - 31	A2 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
32 - 34	P2 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
35 - 37	A2S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
38 - 40	P2S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
41 - 43	A3 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
44 - 46	P3 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
47 - 49	A3S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
50 - 52	P3S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
53 - 55	A3S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0

<u>Card</u>	<u>Data Read</u>	<u>Format</u>
56 - 58	P3S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
59 - 61	A4 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
62 - 64	P4 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
65 - 67	A4S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
68 - 70	P4S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
71 - 73	A5 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
74 - 76	P5 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
77 - 79	A5S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
80 - 82	P5S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
83 - 85	A6 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
86 - 88	P6 (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
89 - 91	A6S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
92 - 94	P6S (I), I=1, 17	5E16.7/5E16.7/4E16.7, 3F10.0
95	N1, N2, N3, N4, N5, N6	6I1
96	EA6 (I), I=1, 6	8F10.0
97	EA6A (I), I=1, 6	8F10.0
98	VKM (I), I=1, 8	8F10.0
99	VKM9	8F10.0
100	TEMP (I), I=1, 8	8F10.0
101	EX	8F10.0
102 - 109	(FIN(I,J), J= 1, 8), I= 1, 7	8F10.0
110 - 118	(COMP(J,I), I=1, 14), J=1, 5	8F10.0/6F10.0
119	IPRNT, TIME, DT, DPRNT	I5, 3F10.0
120-(120+NCHNG)	ICH(NCHNG), IVS(NCHNG), DL(NCHNG), TME, TVL	2I5, 3F10.0
120+NCHNG+1	Blank	

APPENDIX F

Steady State Simulation--Program Listing and Output

U

273

275

```

230      ISTE=3
      IV=4
      DO 231 I=1,14
      A(I)=A04(I)+AF2(I)+A01(I)
      231 P(I)=A04(I)+AF2(I)
      CALL WFSSEL
      C      NITRATOR 3
      IV=5
      IV=7
      234 P(I)=A04(I)+A01(I)
      A(I)=A04(I)+A01(I)
      234 P(I)=A01(I)
      CALL NITSEP
      C      NITRATOR 4
      IV=6
      ISTE=4
      IV=8
      235 P(I)=A04(I)+A05(I)+A01(I)
      A(I)=A04(I)+A05(I)+A01(I)
      235 P(I)=A04(I)+A05(I)
      CALL NITSEP
      C      NITRATOR 5
      IV=11
      IV=7
      ISTE=5
      DO 236 I=1,14
      A(I)=A04(I)+A06(I)+A01(I)
      236 P(I)=A04(I)+A06(I)
      CALL NITSEP
      C      NITRATOR 6
      IV=8
      ISTE=6
      IV=13
      236 P(I)=A04(I)+A06(I)+A01(I)
      A(I)=A04(I)+A06(I)+A01(I)
      236 P(I)=A04(I)+A06(I)
      237 F06=AT(1,1)
      CALL NITSEP
      235      WCI=8
      236      WC2=8
      237      WC3=8
      238      WC4=8
      239      WC5=8
      DO 240 I=1,14
      A(I)=A04(I)+A05(I)
      A(I)=A04(I)+A06(I)
      A(I)=A04(I)+A07(I)
      A(I)=A04(I)+A08(I)
      A(I)=A04(I)+A09(I)
      A(I)=A04(I)+A10(I)
      A(I)=A04(I)+A11(I)
      A(I)=A04(I)+A12(I)
      A(I)=A04(I)+A13(I)
      A(I)=A04(I)+A14(I)
      240      CMTIME
      240      MCS=MC+1
      C      NITRATOR 5

```

PROGRAM TMTSM 76/74 OPT=1

```

345      DO12431=1,16
      ARD4(1)=ARD6(1)
      PID4(1)=PID6(1)
      AT1(1)=AT4(1)+ARD6(1)+AT1(1)
      1243 P11(1)=P14(1)+PID6(1)
      14=7
      14=11
      15=15
      CALL MTTSEP
      NITRATOR 6
      15=14
      14=8
      14=17
      DO12432=1,16
      AT1(1)=AT5(1)+AT1(1)
      1243 P11(1)=P15(1)
      CALL MTTSEP
      IF (11*P11(1).GT.1) WRITE (6,7410) ARD6,PID6
      7410 FORMAT(10X) ITERATION FOR STAGE 6/(11*P11(1))
      DO12432=1,16
      IF (ARD6(1).GT.1) ARD6(1)=GT.DEL160T02403
      IF (PID6(1).GT.1) PID6(1)=GT.DEL160T02403
      2402 CONTINUE
      14=9
      IF (11*P11(1).GT.1) WRITE (6,7410) ARD6,PID6
      7410 FORMAT(10X) ITERATION LOOP FOR STAGE 6 COMPLETED
      14=9
      WRITE (6,7410) ARD6,PID6,ARD5,PID5
      C. ARD5,PID5
      7409 FORMAT(11) 14=9, 3)
      GOT02410
      2407 DO 7407 1=1,16
      ARD4(1)=ARD4(1)+FACT6+ARD6(1)+ARD6(1)
      7407 PID4(1)=PID4(1)+FACT6+PID6(1)+PID6(1)
      IF (11*P11(1).GT.1) WRITE (6,7410) ARD6,PID6
      2405 FORMAT(10X) ITERATION LOOP FOR NITRATOR 5 FAILED TO CONVERGE
      STOP
      2410 DO12431=1,16
      IF (ARD4(1).GT.1) ARD4(1)=GT.DEL160T02413
      IF (PID4(1).GT.1) PID4(1)=GT.DEL160T02413
      2411 CONTINUE
      14=8
      IF (11*P11(1).GT.1) WRITE (6,7410) ARD4,PID4
      7409 FORMAT(11) 14=8, 3) ITERATION LOOP FOR STAGE 5 COMPLETED
      C. ARD4,PID4
      GOT02410
      2413 DO 7413 1=1,16
      ARD5(1)=ARD5(1)+FACT5+ARD5(1)+ARD5(1)
      7413 PID5(1)=PID5(1)+FACT5+PID5(1)+PID5(1)
      IF (11*P11(1).GT.1) WRITE (6,7410) ARD5,PID5
      2416 FORMAT(10X) ITERATION LOOP FOR NITRATOR 4 FAILED TO CONVERGE
      STOP
      2417 NC=944.1
  
```

11/15/74 16.36.10.

FTN 4.1-PSR367

PROGRAM INTS= 74/76 OPT=1

```

400 C *****
      IM=4
      ITCF=4
      IV=0
      N1221=1.14
      A104(1)=A104(1)
      A104(1)=A104(1)
      A111(1)=A111(1)+A104(1)+A104(1)
      A111(1)=A111(1)+A104(1)+A104(1)
      CALL NITCED
      GOT02423
      N1221=1.14
      IF (A104(1)=A104(1)) A104(1)=A104(1)+A104(1)
      IF (A104(1)=A104(1)) A104(1)=A104(1)+A104(1)
      2421 CONTINUE
      N1221=1
      IF (A104(1)=A104(1)) A104(1)=A104(1)+A104(1)
      2422 CONTINUE
      2423 NO 2423 1.14
      2424 A104(1)=A104(1)+A104(1)+A104(1)
      2425 A104(1)=A104(1)+A104(1)+A104(1)
      IF (A104(1)=A104(1)) A104(1)=A104(1)+A104(1)
      2426 A104(1)=A104(1)+A104(1)+A104(1)
      2427 A104(1)=A104(1)+A104(1)+A104(1)
      2428 A104(1)=A104(1)+A104(1)+A104(1)
      2429 A104(1)=A104(1)+A104(1)+A104(1)
      2430 A104(1)=A104(1)+A104(1)+A104(1)
      2431 A104(1)=A104(1)+A104(1)+A104(1)
      2432 A104(1)=A104(1)+A104(1)+A104(1)
      2433 A104(1)=A104(1)+A104(1)+A104(1)
      2434 A104(1)=A104(1)+A104(1)+A104(1)
      2435 A104(1)=A104(1)+A104(1)+A104(1)
      2436 A104(1)=A104(1)+A104(1)+A104(1)
      2437 A104(1)=A104(1)+A104(1)+A104(1)
      2438 A104(1)=A104(1)+A104(1)+A104(1)
      2439 A104(1)=A104(1)+A104(1)+A104(1)
      2440 A104(1)=A104(1)+A104(1)+A104(1)

```

11/15/74 16.30.10.

FTN 4.10P50367

PROGRAM TMSCTM 74/74 JBT=1

```

444      WRITE (A, 7409) ARD3, PUD3, ARD2, PUD2
         C, ARD20, PUD20
         GOTD2444
2637 DO 7677 I=1,14
      ARD7(1)=ARD70(1)+FACT3*(ARD3(1)-ARD30(1))
2637 PUD7(1)=PUD70(1)+FACT3*(PUD3(1)-PUD30(1))
      IF (MC).LT.MC160T02442
         WRITE (6, 7444)
2634 FORMAT (50-0 ITERATION LOOP FOR MITRATOR 2 FAILED TO CONVERGE)
2632 STOP
2632 MC=MC7+1
         C
         MITRATOR 2
         ISTEP=2
         IN=1
2624
         DO 1217 J=1,14
           ARD70(1)=ARD7(1)
           PUD70(1)=PUD7(1)
           ARD7(1)=ARD7(1)+ARD7(1)+ARD7(1)
1217 PUD7(1)=PUD7(1)+PUD7(1)
           CALL MTSCEP
           GOTD2442
2644 DO 7644 I=1,14
      IF (ARD7(1)-ARD70(1)).GT.DEL160T02443
      IF (PUD7(1)-PUD70(1)).GT.DEL160T02443
2641 CONTINUE
           MC1=8
           GOTD2449
2647 DO 7647 I=1,14
      ARD2(1)=ARD20(1)+FACT2*(ARD2(1)-ARD20(1))
2647 PUD2(1)=PUD20(1)+FACT2*(PUD2(1)-PUD20(1))
      IF (MC1).LT.MC160T02442
         WRITE (6, 7444)
2644 FORMAT (50-0 ITERATION LOOP FOR MITRATOR 1 FAILED TO CONVERGE)
         STOP
2642 MC1=MC1+1
         C
         MITRATOR 1A
         ISTEP=1
         IN=1
2624
           DO 1207 J=1,14
             ARD20(1)=ARD2(1)
             PUD20(1)=PUD2(1)
             ARD2(1)=ARD2(1)+ARD2(1)
1207 PUD2(1)=PUD2(1)
             PUD2(1)=PUD2(1)+PUD2(1)
             CALL MTSCEP
             C
             MITRATOR 1B
             IN=2
             DO 1207 J=1,14
               ARD1(1)=ARD1(1)+ARD1(1)
1207 PUD1(1)=PUD1(1)+PUD1(1)
             CALL MTSCEP
             GOTD2442

```



```

745      CUM1=ARRAY(1,6)
      TATM=TATM+(NF(1,ISTG)-OFF(1,ISTG)+ARR(1,ISTG)+PAR(1,ISTG))
      C ATOM(MATH,1)
      IF(ISTG.EQ.3) SUM1=SUM1+ARRAY(1,5)
      IF(ISTG.EQ.1) GOT04073
      SUM1=SUM1+ARRAY(1,2) +ARR(1,1)
      IF(1,FO,10) CUM1=SUM1+0.1*P101
      GOT04075
747      SUM1=SUM1+NF(1,ISTG)-1+OFF(1,ISTG-1)
748      IF(ISTG.EQ.4) SUM1=SUM1+ARR(1,ISTG+1)+PAR(1,ISTG+1)
749      TATM=TATM+SUM1+ATOM(MATH,1)
      D04574L=1+4
      CUM=CUM(1,1)+C65(1,1+1,1)
      IF(ISTG.EQ.1) OFF(1,ISTG-1)+SUM-SUM+C65(1,2+1,1)
      IF(MATH.FO.3) ARR(1,1.EQ.2) TATM=TATM+OFF+SUM
7476      TATM=TATM+SUM+C65(MATH,1)
      OFF=TATM-TATM
7477      WRITE(6,4001) (MATH,1,1+1,2) TATM,TATM+OFF
7478      CONTINUE
      IV=3
      IV=3
      D04499ISTG=1+6
      IV=IV+1
      IV=IV+1
      IV=IV+1
      WRITE(6,4009) IV
7479      FORMAT(4009) 1V
      WRITE(6,4005)
      D0494MATH=1+5
      TATM=0.
      TATM=0.
      D04499N=1+4
7480      TATM=TATM+C65(MATH,1)+C65(1V,1)
      IF(MATH.FO.3) TATM=TATM+ARR+C65(1V,2)
      D04497I=1+14
      TATM=TATM+ARRAY(1,14)+ATOM(MATH,1)
      IF(ISTG.EQ.1) TATM=TATM+(NF(1,ISTG)-1)+OFF(1,ISTG-1)+ATOM(MATH,1)
      C 1)
      IF(ISTG.EQ.4) TATM=TATM+ARR(1,ISTG+1)+PAR(1,ISTG+1)
      C ATOM(MATH,1)
      IF(ISTG.EQ.1) OFF(1,ISTG-1)+GOT04096
      TATM=TATM+ARR(1,ISTG)+PAR(1,ISTG)+ATOM(MATH,1)
      GOT04005
7481      IF(ISTG.FO.1) ARR(1,1.EQ.10) TATM=TATM+PAR+ATOM(MATH,1)
7482      TATM=TATM+ARR(1,10)+OFF(1,10)+ATOM(MATH,1)
7483      CONTINUE
      GIP=TATM-TATM
7484      WRITE(6,4001) (MATH,1,1+1,2) TATM,TATM+OFF
      IF(ISTG.EQ.1) ARR(1,ISTG+1)+C65(1,1)
      IV=IV+1
      IV=IV+1
      WRITE(6,4009) IV
      WRITE(6,4005)
      D04499MATH=1+5
      TATM=0.
      TATM=0.
      D04497I=1+14
      TATM=TATM+ARR(1,10)+OFF(1,10)+ATOM(MATH,1)

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11/15/74 16.38.10.

FTN 4.1:PSR367

PROGRAM TMTSSM 74/74 OPT=1

```

      WTH=0.
      CTM=P.
      SUM=0.
      SPACTD=SPA*SPP
      PCTMR=(TAMP*TMQR)/SPACTD*100.
      PCTMRD=TAMP/SPA*100.
      PCTD=(ARP(1)*ARR(4))*MM(1)*100./TAMP
      DO6C29J=1,4
      TOL=TOL+FIN(6,J)
      SULP=SULP+FIN(5,J)
      WTH=MM+FIN(1,J)+FIN(2,J)
      STN=STN+FIN(4,J)
      CTM=CTM+TOL+CSL+SULP+WTH*MM+CSM*STN/(TOL+VIEL*MM(5)*.0001)
      DO6A70I=1,6
      KEY=0
      I1=KEY
      IJ=KEY
      PFC=0.
      IF (I1.EQ.6)GOTO6072
      I1=1
      DO6A71J=1,IJ,2
      K=(J+1)/2
      6031 REC=REC+ARR(J,I)*PIR(J,I)
      6032 IF (I1.EQ.1)GOTO6033
      FME=1.*TMTI
      IF (KEY.EQ.1)FDM=0.
      GOTO6034
      6033 FDM=0.
      IY=1
      DO6A75J=1,IJ,2
      K=(J+1)/2
      6035 FDM=FDM+PFC(J,IY)*AF(J,IY)
      6036 OUTM=0.
      DO6A76J=1,IJ,2
      K=(J+1)/2
      6036 OUTM=OUTM+PFC(J,I)*AF(J,I)*PIR(J,I)
      IF (KEY.FQ.1)GOTO6030
      KEY=1
      SRA(1)=AR
      GOTO6029
      6030 SRA(1)=AR
      6030 CPUTIME
      C
      COMPUTATION OF ACTUAL ACIDITY
      DO6A80I=1,4
      TMOLES=ARP(9,I)
      TLRS=TMOLES*MM(9)
      DO6A81J=1,14
      TMOLES=TMOLES+ARR(J,I)
      TLRS=TLRS+ARR(J,I)*MM(I)
      6041 AN(I)=140.*ARR(9,I)*MM(9)/TLRS
      AS(I)=100.*ARR(9,I)*MM(9)/TLRS
      ATQ(I)=ARR(9,I)/(ARR(11,I)+ARR(14,I))*MM(11)/TLRS
      AWS(I)=ARR(12,I)/TMOLES
      PWS=10P*ARR(12,I)/TLRS*MM(12)
      TM(I)=AM(I)*8.4559*PWS
      VS(I)=AS(I)*0.7718*PWS

```

TMTSS 758
 TMTSS 759
 TMTSS 760
 TMTSS 761
 TMTSS 762
 TMTSS 763
 TMTSS 764
 TMTSS 765
 TMTSS 766
 TMTSS 767
 TMTSS 768
 TMTSS 769
 TMTSS 770
 TMTSS 771
 TMTSS 772
 TMTSS 773
 TMTSS 774
 TMTSS 775
 TMTSS 776
 TMTSS 777
 TMTSS 778
 TMTSS 779
 TMTSS 780
 TMTSS 781
 TMTSS 782
 TMTSS 783
 TMTSS 784
 TMTSS 785
 TMTSS 786
 TMTSS 787
 TMTSS 788
 TMTSS 789
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 TMTSS 792
 TMTSS 793
 TMTSS 794
 TMTSS 795
 TMTSS 796
 TMTSS 797
 TMTSS 798
 TMTSS 799
 TMTSS 800
 TMTSS 801
 TMTSS 802
 TMTSS 803
 TMTSS 804
 TMTSS 805
 TMTSS 806
 TMTSS 807
 TMTSS 808
 TMTSS 809
 TMTSS 810
 TMTSS 811

```

010 6040 TMS(1)=ACS(1)+T4(1)+0.7792
      NTOS14=AV(10.11)/(AV(11.11)+AV(14.11))
      NTOS15=AV(10.61)/(AV(11.61)+AV(14.61))
      ANSL14=AV(12.11)/(AV(9.11)+AV(11.11)+AV(12.11)+AV(14.11))
      ANSL15=AV(12.61)/(AV(9.61)+AV(11.61)+AV(12.61)+AV(14.61))
      C
      COMPUTATION OF NO DENSITY
      NOGAS1=1.04
      TLPS=NO(10)+AKR(10.1)
      TUN=NO(10.11)+RMO(10)
      NOGASJ=1.04
      TLPS=TLPS+AKR(J.1)+RMO(J)
      TUN=TUN+AKR(J.1)+RMO(J)
      6045 DMOPUS(1)=TLPS/TUN
      6045 WRITE(4,490)YIELD,CRUMF+CMT+CTF+SPA+SPP+SPACID+PCTMB+PCTMBD,
      C PCTN,
      1 (1.5+ACT)+SMP(11)+AM(11)+AS(11)+TMS(11)+TAS(11)+RHMOS(11)+1.16)
      6050 FORMAT(11SESSSIMPMDRY+OBYIELD=0.77.3.0 MOLE PCT TOL CONVERSION T
      CD TMT/
      1 0 LBS/NO CRUMF TMT=0.77.2.0 WT PCT DMT IN CRUDE TMT=0.77.4.4/
      2 0 RAW MATERIALS COST, G/LR OF A-TMT=0.77.6.6/
      3 0 PERCENT ACID FLOW, LBS/MO/RAW+ACID DM.0.77.6.4/
      4 6X+NOG. DM.0.77.6.4/6X+TOTAL.0.77.6.0 WT PCT TOTAL MB=0.77.6.4/
      5 0 WT PCT DISSOLVED NO=0.77.6.4/
      6 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
      7 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
      8 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
      9 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
      10 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
      11 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
      12 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
      13 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
      14 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
      15 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
      16 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
      17 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
      18 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
      19 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
      20 0 WT PCT DMT IN DISSOLVED NO=0.77.6.4/0.77.6.4/0.77.6.4/
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PROGRAM	TNTS1M	74/76	OPT=1	FTW 4.1+PSR367	11/15/74	16.30.20.	PAGE	10
970	GOTN5				TNTSS	067		
	55	O=O*ENTH(A7A,P7A,T7A)+ENTH(A107,P107,TSEP3)-ENTH(A30,P30,T30)			TNTSS	068		
		GOTN57			TNTSS	069		
	56	O=O*ENTH(A73,P73,TSEP3)+ENTH(A107,P107,TSEP5)+ENTH(A30,P30,T30)			TNTSS	070		
		C ENTH(A107,P107,TSEP4)-ENTH(A4,P4,T4)			TNTSS	071		
975	GOTN58				TNTSS	072		
	57	O=O*ENTH(A74,P74,TSEP4)+ENTH(A107,P107,TSEP6)+ENTH(A30,P30,T30)			TNTSS	073		
		C ENTH(A107,P107,TSEP5)-ENTH(A5,P5,T5)			TNTSS	074		
	GOTN59				TNTSS	075		
	58	O=O*ENTH(A75,P75,TSEP5)+ENTH(A107,P107,TSEP6)-ENTH(A6,P6,T6)			TNTSS	076		
980	RTU(1)=0./752				TNTSS	077		
	59	WRITE(6,61) (1,RTU(1),T=1.0)			TNTSS	078		
	61	FORMAT(1,0)NITRATOR HEAT DUTIES=61,0NITRATOR=51,0BTU=7			TNTSS	079		
		1 (11,19,F14.0)			TNTSS	080		
		60 TO 4001			TNTSS	081		
985	END				TNTSS	082		

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
S153 TMTSIM

VARIABLES	SN	TYPE	DELOCATION	14701 AB	REAL	ARRAY	11/15/74	16.36.10.	PAGE
304 AAS	0	REAL	AC	14701 AB	REAL	ARRAY	11/15/74	16.36.10.	PAGE
0 AF	0	REAL	SOLV	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
0 AF1	16	REAL	SOLV	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
34 AF3	52	REAL	SOLV	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
70 AF5	106	REAL	SOLV	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
0 AI	0	REAL	INPUT	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
124 A10	0	REAL	SOLV	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
124 A101	142	REAL	SOLV	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
160 A103	176	REAL	SOLV	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
216 A105	232	REAL	SOLV	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
112 A14	14543	REAL	SOLV	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
14544 AHC	113	REAL	Z	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
14545 AHECOV	73	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
74 AHWATL	61	REAL	Z	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
46 AK12	53	REAL	Z	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
67 AKW	54	REAL	Z	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
59 AKW4	51	REAL	Z	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
52 AKG5	57	REAL	Z	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
44 AK4	101	REAL	Z	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
17344 AN	15741	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
16705 ANSLA	14706	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
14616 AT	17354	REAL	X	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
0 AV	16852	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
250 A10	16160	REAL	AC	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
250 A101	15271	REAL	SOLV	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
17034 A1020	266	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
17052 A1030	304	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
17070 A1040	322	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
17106 A1050	340	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
17124 A1060	356	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
0 A1A1	0	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
14 A1A1	16	REAL	X	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
52 A2	34	REAL	X	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
70 A25	34	REAL	AC	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
52 A7A1	106	REAL	AC	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
70 A7A1	124	REAL	X	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
160 A6	142	REAL	X	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
174 A65	106	REAL	AC	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
124 A51	214	REAL	AC	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
250 A6	232	REAL	X	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
266 A65	142	REAL	AC	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
17024 A7100	14741	REAL	AC	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
17420 C0MP	14652	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
14653 C0NIDE	16	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
12177 C5N	12175	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
12174 C7L	14670	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
6 C6L	12176	REAL	VECTOR	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
14645 C1F	34	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
1124 C40	14714	REAL		15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE
12201 C6P	1134	REAL	SOLV	15471 AFLBS	REAL	ARRAY	11/15/74	16.36.10.	PAGE

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FTN 4.1-PSM367 11/15/74 16.30.10.

74/74 OPT=1

PROGRAM INTSIN

STATFMT LABELS

7624	1710	7453	1720	7701	1730
7730	1740	0	2300	0	2402
7200	2403	7114	2404	13174	2405
7217	2410	0	2411	7262	2412
7263	2413	13230	2416	7304	2420
0	2421	7347	2422	7330	2423
13264	2424	7404	2430	0	2431
7447	2432	7430	2433	13320	2434
7471	2440	0	2441	7527	2442
7510	2443	13332	2444	7565	2450
13344	2451	0	3213	0	3214
0	3221	0	3233	0	3234
0	3243	0	3253	0	3263
0	3403	0	3413	0	3423
0	3433	0	3443	13150	3600
13204	3401	13242	3602	13270	3603
13167	3444	13140	3610	0	3900
7401	3901	7654	3902	7701	3903
0	3905	13153	4003	13363	4001
13400	4002	13426	4003	13447	4004
13471	4005	14161	4009	14002	4010
14074	4011	14122	4012	14144	4013
14172	4044	0	4010	0	4071
0	4072	10571	4073	0	4074
10574	4075	14225	4080	14242	4091
14233	4085	14202	4086	0	4090
0	4001	0	4092	0	4093
10743	4004	10752	4095	0	4096
0	4007	0	4098	13542	4100
13560	4101	0	4102	13600	4103
13131	4207	14200	5000	0	5001
0	5002	0	5003	11077	5010
0	5011	0	5012	0	5013
13515	4000	6274	6001	13606	6003
13552	4004	10420	6000	11154	6009
0	4017	0	6018	0	6019
0	4020	0	6025	0	6027
11112	4020	0	6029	0	6030
0	4031	11137	6032	11346	6033
11165	4934	0	6035	0	6036
11014	4934	0	6040	0	6041
0	4045	0	6046	14361	6050
0	4147	0	0000	0	0000

INACTIVE

INACTIVE

BLOCKS	LENGTH
FLAG	4
DATA	17
INPUT	34
ITCP	28
NOO	14
FO	22
PC	112
AC	214
COLV	210
NUM	710
VECTOR	11
	10

FTN 4.10PS0367 11/15/74 16.30.10. PAGE 24

74/74 OPT=1

PROGRAM INTSIN

COMMON BLOCKS LENGTH
7 75
PAR 68

STATISTICS

PROGRAM LENGTH 125149
BUFFER LENGTH 61639
COMMON LENGTH 70148
5453
9171
1548

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CURROUTINE NITSEP
  DIMENSION AIRQ(14),AIRP(14),AF(14),PIR(14),PPI(14),PF(14)
  COMMON/FLAG/IFLG(6)
  COMMON/VFCTNO/ITYPE,IPONT,NC,ISTGE,IN,IV,DEL,IE,IAFT,ICHECK
  COMMON/SCNLY/AF(14,6),AP(14,6),APR(14,6),PF(14,6),PIR(14,6),
  C PIR(14,6),TSEP(6),
  C PIR(14,6),C16(14),C19(14),SOL(14)
  C AF(14,6),EAD(6),RATES(14,10),FACD(6),YELLOW(14)
  COMMON/PP/PV(14,15)
  COMMON/AC/AV(14,15)
  COMMON/NITSP/AT(14),PI(14)
  COMMON/INPUT/AI(17),PI(17)
  EQUIVALENCE (AF(14,6),AP(14,6),APR(14,6),PF(14,6),PIR(14,6),
  C PIR(14,6),C16(14),C19(14),SOL(14))
  C PIR(14,6)
  ICOMP=0
  IV=IV+1
  DO 17 I=1,14
    AI(I)=AV(I,IV)
    PI(I)=PV(I,IV)
    ITYPE=1
    CALL VFSEL
    IF (ICOMP) 19,19,21
    IF (ICOMP-NC) 25,25,26
    CONTINUE
    IF (IPONT.EQ.1) 19,19,19
    IF (ISTGE.IE.10)
    C ICOMP=INTERNAL RECYCLE FOR STAGE,12/0 AIR=14F0.3/0 PIR=
    C 14F0.3/
    DO 11 I=1,14
      IF (AIR(I).ISTGE)-AIR(I)-DEL130.30.29
      IF (AIR(I).ISTGE)-PIR(I)-DEL131.31.29
    CONTINUE
    RETURN
  19 WRITE(6,27)ISTGE,NC
  FORMAT(12HINTERNAL RECYCLE LOOP FOR STAGE,12. 23H FAILED TO CONV
  GEDE 14.13. 11H ITERATIONS)
  IF (ISTGE)=1
  RETURN
  20 CONTINUE
  19 CONTINUE
  ICOMP=ICOMP+1
  IF (ISTGE.NE.2) GO TO 5
  IF (IAFT.F0.0) 5059
  IV=IV
  IV=15
  DO 11 I=1,14
    AI(I)=AI(I)+YELLOW(I)
    PI(I)=PI(I)
    CALL VFSEL
    IV=IV+1
    DO 11 I=1,14
      AIR(I)=AIR(I)+ISTGE
      PIR(I)=PIR(I)+ISTGE
  11
  50
  55
  75

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40 IF (11575.NF.11)GOTO36
   IF (11575.FO.01)GOTO17
   D0441=1.14
   A1(1)=A1(11)+A1R0(1)
   P1(1)=P1(11)+P1R0(1)+P1(1).15)
   GOTO45
64 D0441=1.14
   A1(1)=A1(11)+A1R0(1)
   P1(1)=P1(11)+P1R0(1)+P1(1)
   GOTO45
76 D0471=1.14
   A1(1)=A1(11)+A1R0(1)
   P1(1)=P1(11)+P1R0(1)
45 IYPE=9
   CALL VFSEL
   GOTO49
   END
TMTSS 940
TMTSS 941
TMTSS 942
TMTSS 943
TMTSS 944
TMTSS 945
TMTSS 946
TMTSS 947
TMTSS 948
TMTSS 949
TMTSS 950
TMTSS 951
TMTSS 952
TMTSS 953
TMTSS 954
TMTSS 955
TMTSS 956

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SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
1 HTSFP

VARIABLES	SN	TYPE	DECLARATION
0 AF	0	REAL	ARRAY SOLV
0 AT	0	REAL	ARRAY INPUT
124 ATQ	0	REAL	ARRAY SOLV
124 ATQI	0	REAL	ARRAY SOLV
250 AXD	0	REAL	ARRAY SOLV
6 BEL	0	REAL	VECTOR
1004 FADP	0	REAL	ARRAY SOLV
1012 FOAP	0	REAL	ARRAY SOLV
1020 G15	0	REAL	ARRAY SOLV
1034 G1A	0	REAL	ARRAY SOLV
217 T	0	INTEGER	VECTOR
11 TCHECK	0	INTEGER	VECTOR
7 TF	0	INTEGER	VECTOR
4 TM	0	INTEGER	VECTOR
3 TSTGE	0	INTEGER	VECTOR
5 TV	0	INTEGER	VECTOR
214 TVO	0	INTEGER	VECTOR
774 MO	0	REAL	ARRAY SOLV
374 PF1	0	REAL	ARRAY SOLV
14 P11	0	REAL	ARRAY SOLV
237 P100	0	REAL	ARRAY SOLV
8 OV	0	REAL	ARRAY SOLV
644 P101	0	REAL	ARRAY SOLV
1110 CNL	0	REAL	ARRAY SOLV
1270 VELLON	0	REAL	ARRAY SOLV

0 AF1	0	REAL	ARRAY
0 A11	0	REAL	ARRAY
221 A1RO	0	REAL	ARRAY
0 AV	0	REAL	ARRAY
250 A1P1	0	REAL	ARRAY
1126 EAO	0	REAL	ARRAY
1134 EAO	0	REAL	ARRAY
1262 FAD	0	REAL	ARRAY
1036 G16	0	REAL	ARRAY
1072 G19	0	REAL	ARRAY
10 IAF1	0	INTEGER	VECTOR
215 ICOUNT	0	INTEGER	ARRAY
0 IFLG	0	INTEGER	VECTOR
1 IPPMT	0	INTEGER	VECTOR
0 ITYPE	0	INTEGER	VECTOR
220 IVA	0	INTEGER	VECTOR
2 NC	0	INTEGER	VECTOR
374 PF	0	REAL	ARRAY
21 P1	0	REAL	ARRAY
520 P1P	0	REAL	ARRAY
520 P1P1	0	REAL	ARRAY
644 P1P	0	REAL	ARRAY
1142 RATES	0	REAL	ARRAY
770 TSEP	0	REAL	ARRAY

FILE NAMES
TAPEN
WDF
FMT

EXTERNALS
VFCSEL
TYPE ARG
0

INLINE FUNCTIONS
TYPE ARG
1 INTRIN

STATEMENT LABELS

0 17	62 19
0 21	0 25
203 27	62 29
0 31	0 35
131 37	4 40
0 44	155 45
0 47	103 50

INACTIVE
INACTIVE

INACTIVE

0 20
56 26
0 30
144 36
0 41
0 46
166 506
FMT

COMMON
BLOCKS
FLAG
VECTOR
CNL
PC
AC
NTSP

LENGTH
6
18
710
210
210
28

PAGE 4

FTN 4.1-PS367 11/15/76 16.30.32.

76/74 OPT=1

COMROUTINE NITSEP

COMMON BLOCKS LFM5TH
INPUT 74

STATISTICS

PROGRAM LENGTH 255H
COMMON LENGTH 2270H

173
179H

CURRENT VESSEL 74/74 OPT=1

```

60      AL=A(13)-A(14)
        P18=P(18)
        ICOUNT=0
        G1=F1(14)
        G3=F3(14)
        G4=F4(14)
        G5=F5(14)
        G6=F6(14)
        G7=F7(14)
        G8=F8(14)
        G9=F9(14)
        G10=F10(14)
        TREL=TF*P(14)+273.3
        IF (I1TYPE)140,140,140
141      FV=V*V*V*V*V*V*V*V*V*V
        GOTO162
142      FV=C*V*V*V*V*V*V*V*V*V*V
        ICOUNT=ICOUNT+1
        IF (ICOUNT-NC) 163,163,164
143      CONTINUE
        IF (A9-L1-L1) A9=1.
        DO161I=1,22
144      V0(I)=V(11)
145      IF (A1-L1-L1) A1=1.
        A13=9.
        A14=AL
        GOTO172
146      A13=AL
        A14=9.
        CONTINUE
        A11=A504-A14
        IF (A11-L1-L1) A11=1.
        COMPUTE TOTAL FLOWS
        A9=9.
        P9=9.
        DO199I=1,P
        A9=A9+A95(I*(1))
        P9=P9+A95(I*(12))
199      P9=P9+A95(I*(10))
        IF (A9-L1-L1) A9=9.
        IF (P9-L1-L1) P9=1.
        AT=A9+A95(I*(9))-A95(A11)+A95(A12)+A13+A14
        IF (AT-L1-L1) AT=1.
        COMPUTE DENSITIES
        Q4=A1/P*Q1+Q2/P*Q2+Q3/P*Q3+Q4/P*Q4+Q5/P*Q5+Q6/P*Q6+Q7/P*Q7+Q8/P*Q8
        C A11/P*Q1+Q2/P*Q2+Q3/P*Q3+Q4/P*Q4+Q5/P*Q5+Q6/P*Q6+Q7/P*Q7+Q8/P*Q8
        Q9=P1/P*Q1+Q2/P*Q2+Q3/P*Q3+Q4/P*Q4+Q5/P*Q5+Q6/P*Q6+Q7/P*Q7+Q8/P*Q8
        C P1/P*Q1+Q2/P*Q2+Q3/P*Q3+Q4/P*Q4+Q5/P*Q5+Q6/P*Q6+Q7/P*Q7+Q8/P*Q8
        IF (Q4-L1-L1) Q4=1.
        IF (Q9-L1-L1) Q9=1.
        IF (I1TYPE)111,111,12
        F4=Q4/Q4+Q9
11      GOTO13

```

TNTSS 1011
TNTSS 1012
TNTSS 1013
TNTSS 1014
TNTSS 1015
TNTSS 1016
TNTSS 1017
TNTSS 1018
TNTSS 1019
TNTSS 1020
TNTSS 1021
TNTSS 1022
TNTSS 1023
TNTSS 1024
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TNTSS 1066
TNTSS 1067

```

115      12  FA=.795
116      13  FP=1.-FA
117      C  COMPUTE MOLE FRACTIONS
118      AT1=1./AT
119      X13=A13*ATI
120      X1=A1*ATI
121      X2=A2*ATI
122      X5=A5*ATI
123      X6=A6*ATI
124      X7=A7*ATI
125      X10=A10*ATI
126      COMPUTE XEQ
127      PPZ=-1.62+.01023*TKEL-1.000*113-7.716*(X1+X2)-0.452*(X5+X6)-
128      C  5.592*19
129      IF (PP.GT.300.) PP=300.
130      IF (PP.LT.-250.) PP=-250.
131      XEQ=1E+000
132      C  COMPUTE ETA
133      IF (11*PP) 15,15,16
134      ETAB=FVW*FP*AKNA
135      ETAP=FVW*FP*AKNP
136      ETAL=1./11./ETAP+1./11./ETAB*(XEQ+1)
137      ETATL=FVW*FP*AKNATL
138      C  COMPUTE D
139      ZA=ETA/PMO
140      ZB=ETA/PMO
141      D1=ZA*P1-ZB*A1
142      D2=ZA*P2-ZB*A2
143      D3=ZA*P3-ZB*A3
144      D4=ZA*P4-ZB*A4
145      D5=ZA*P5-ZB*A5
146      D6=ZA*P6-ZB*A6
147      D7=ZA*P7-ZB*A7
148      D8=ZA*P8-ZB*A8
149      D10=ETATL*P10/PMO
150      GO TO 17
151      D1=0.
152      D2=0.
153      D3=0.
154      D4=0.
155      D5=0.
156      D6=0.
157      D7=0.
158      D8=0.
159      D10=0.
160      CONTINUE
161      C  COMPUTE M
162      A1W=A11+A12+A13+A14+A15+A16+A17+A18
163      AMW=AT*EQ+A-A1W-01-02-03-04-05-06-07-08
164      IF (1*PP) 17,17,18
165      C  WRITE (6,304) AT,PT,AMB,PMO,A1W,AMW,XEQ,A1,D1,D2,D3,D4,D5,D6,D7,D8
166      C  304
167      C  304  FORMATTED AT,PT,AMB,PMO,A1W,AMW,XEQ,A1,D1,D2,D3,D4,D5,D6,D7,D8
168      C  304  C = D1-D10, OF 12.5)
169      C  COMPUTE GAMMA
170      GAM=1./PMO

```

TMTSS 1068
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 TMTSS 1123
 TMTSS 1124
 TMTSS 1125
 TMTSS 1126
 TMTSS 1127
 TMTSS 1128
 TMTSS 1129
 TMTSS 1130


```

400      DO10A1=1.27
        IF (ABS(V(1)-V0(1))-OLA)/100.100.173
          CONTINUE
100      IF (IPONT-EO.1) WRITE(6,9010)IV-FACT-0.8
9010      FORMAT(' VESSEL-0.13.0 CONVERGED. FACT =-F10.5-SE-00 -F0.5/
          C 110710.01
160      DO10A1=1.14
          A(1)=0.
          P(1)=0.
175      DO10A1=1.0
          A(1)=V(1)
          P(1)=V(1)+12)
186      IF (AL1/100.191.191
190      A(1)=0.
          A(14)=AL
          GOT0192
191      A(1)=AL
          A(14)=0.
192      CONTINUE
          A(9)=00
          A(11)=AS04-A(14)
          A(12)=A12
          P(0)=00
          P(10)=P10
          IF (IV.F0.15) GOT0150
          GO(IV)=0
          G15P=0.07.7.000
          G15P=G15P+7.0006
          G15(IV)=G15P
          G16(IV)=00.670(1.-00)
          G18(IV)=07
          G19(IV)=010
          S0L(IV)=E04
          IF (ITYPE) 00.00.01
          70=0.
          70=0.
          00=21=1.0
          70=70.0(11)+CP(11)
          00=31=1.14
          70=70.0(11)+CP(11)
          00=61=1.10
          70=70.0(11)+00(11)
          TSEP(15EP)=TEMP(100)+20/74
          IF (IE1109.109.110
100      CONTINUE
          P(1)=1./PT
          X7=A70ATI
          X8=A80ATI
          X7=A70ATI
          X11=A110ATI
          X8=A80ATI
          X12=A120ATI
          X13=A130ATI
          V1=010ATI
          V2=020ATI
          V3=030ATI
          V4=040ATI

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SUBROUTINE VESSEL 74/74 OPT=1

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
1 VESSEL

VARIABLES	SW	TYPE	REL. LOCATION	ARRAY	REL	ARRAY	SOLV
3516 A	0	AF	INPUT	ARRAY	REAL	ARRAY	SOLV
0 A7	0	AF	INPUT	ARRAY	REAL	ARRAY	INPUT
124 A10	11	AF	INPUT	ARRAY	REAL	ARRAY	INPUT
11 A110	11	AF	INPUT	ARRAY	REAL	ARRAY	INPUT
15 A112	15	AF	INPUT	ARRAY	REAL	ARRAY	INPUT
17 A116	17	AF	INPUT	ARRAY	REAL	ARRAY	INPUT
1 A12	1	AF	INPUT	ARRAY	REAL	ARRAY	INPUT
3 A14	3	AF	INPUT	ARRAY	REAL	ARRAY	INPUT
5 A16	5	AF	INPUT	ARRAY	REAL	ARRAY	INPUT
7 A18	7	AF	INPUT	ARRAY	REAL	ARRAY	INPUT
112 A24	112	AF	INPUT	ARRAY	REAL	ARRAY	INPUT
2402 ANFOQV	2402	AF	INPUT	ARRAY	REAL	ARRAY	INPUT
3144 ANFO2	3144	AF	INPUT	ARRAY	REAL	ARRAY	INPUT
77 ANFO4	77	AF	INPUT	ARRAY	REAL	ARRAY	INPUT
74 ANFO6	74	AF	INPUT	ARRAY	REAL	ARRAY	INPUT
3242 AK1	66	AK12	INPUT	ARRAY	REAL	ARRAY	INPUT
46 AK15	53	AK15	INPUT	ARRAY	REAL	ARRAY	INPUT
3295 AK4	50	AK4	INPUT	ARRAY	REAL	ARRAY	INPUT
52 AK65	52	AK65	INPUT	ARRAY	REAL	ARRAY	INPUT
60 AK8	60	AK8	INPUT	ARRAY	REAL	ARRAY	INPUT
3572 AN	3572	AN	INPUT	ARRAY	REAL	ARRAY	INPUT
3314 A01	11	AS04	INPUT	ARRAY	REAL	ARRAY	INPUT
7200 A11	3444	A11	INPUT	ARRAY	REAL	ARRAY	INPUT
3444 A11	3385	A11	INPUT	ARRAY	REAL	ARRAY	INPUT
3424 A12	3426	A12	INPUT	ARRAY	REAL	ARRAY	INPUT
3430 A16	3432	A16	INPUT	ARRAY	REAL	ARRAY	INPUT
3432 A18	0	A1	INPUT	ARRAY	REAL	ARRAY	INPUT
12 A12	3166	A14	INPUT	ARRAY	REAL	ARRAY	INPUT
1 A2	1	A2	INPUT	ARRAY	REAL	ARRAY	INPUT
3 A4	5	A6	INPUT	ARRAY	REAL	ARRAY	INPUT
7 A8	3253	A	INPUT	ARRAY	REAL	ARRAY	INPUT
3253 A	3310	A1	INPUT	ARRAY	REAL	ARRAY	INPUT
3254 C	3261	C	INPUT	ARRAY	REAL	ARRAY	INPUT
3261 C	3247	C4003	INPUT	ARRAY	REAL	ARRAY	INPUT
3247 C4003	3255	C45207	INPUT	ARRAY	REAL	ARRAY	INPUT
3255 C45207	3246	C47504	INPUT	ARRAY	REAL	ARRAY	INPUT
3246 C47504	3243	C402	INPUT	ARRAY	REAL	ARRAY	INPUT
3243 C402	3300	C4	INPUT	ARRAY	REAL	ARRAY	INPUT
3300 C4	3344	C12	INPUT	ARRAY	REAL	ARRAY	INPUT
3344 C12	3301	C1	INPUT	ARRAY	REAL	ARRAY	INPUT
3301 C1							

VARIABLES	SN	TYPE	RELOCATION	33-42	CIP	REAL	ARRAY	VECTOR	FTN 4.1-050367	11/15/74	12.58.40.	PAGE	14
3303 C10	REAL			3302 C1P	REAL								
3306 C11	REAL			3307 C12	REAL								
3313 C21	REAL			3312 C22	REAL								
3330 C4	REAL			3326 C5	REAL								
3327 CSP	REAL			3331 C6	REAL								
3562 PD	REAL			6 DEL	REAL								
34 PM	REAL			2403 DLA	REAL								
3363 N0N	REAL			3220 01	REAL								
3230 N10	REAL			3221 02	REAL								
3222 03	REAL			3223 04	REAL								
3224 P5	REAL			3225 06	REAL								
3226 07	REAL			3227 08	REAL								
1126 F40	REAL			1004 EAP	REAL								
3365 F404	REAL			1134 E04	REAL								
1012 EQAP	REAL			3214 ETA	REAL								
3212 FT04	REAL			3213 ETAP	REAL								
3215 FTATL	REAL			3346 EXI	REAL								
71 F10	REAL			62 EZI	REAL								
55 F35	REAL			63 F3V	REAL								
54 F45	REAL			64 F4V	REAL								
65 F55	REAL			66 F65	REAL								
67 F7	REAL			70 E0	REAL								
3233 F	REAL			3176 FA	REAL								
1262 F4CD	REAL			3105 FACT	REAL								
3406 FAR	REAL			3407 FAWI	REAL								
3263 FC	REAL			72 FD	REAL								
3466 FF	REAL			3370 FNG	REAL								
3371 F10	REAL			1367 FLV	REAL								
110 FMAX	REAL			3372 FOG	REAL								
3371 FOGC	REAL			3177 FP	REAL								
3410 FPD	REAL			3411 FP01	REAL								
3414 FR	REAL			3413 FRAC	REAL								
3164 FVCH	REAL			0 F1	REAL								
110 F10	REAL			10 F3	REAL								
34 F35	REAL			20 F4	REAL								
40 F45	REAL			50 F5	REAL								
60 F6	REAL			70 F7	REAL								
100 F8	REAL			120 F9	REAL								
3266 GAMMA	REAL			3150 G1	REAL								
3162 G10	REAL			3275 G10P	REAL								
1020 G15	REAL			3372 G15P	REAL								
1016 G16	REAL			1054 G18	REAL								
1072 G19	REAL			3151 G3	REAL								
3267 G30	REAL			3153 G35	REAL								
3152 G4	REAL			3270 G40	REAL								
3154 G45	REAL			3155 G5	REAL								
3271 G56	REAL			3154 G6	REAL								
3272 G66	REAL			3157 G7	REAL								
3273 G76	REAL			3160 G8	REAL								
3274 G8P	REAL			3161 G9	REAL								
3276 G96	REAL			3142 I	INTEGER								
10 IAT	INTEGER			11 ICHECK	INTEGER								
3147 ICOUNT	INTEGER			7 IE	INTEGER								
12 I11	INTEGER			4 IN	INTEGER								
1 IPWNT	INTEGER			3 ISEP	INTEGER								
3 ISTE	INTEGER			3146 ITR	INTEGER								
8 ITYPE	INTEGER			5 IV	INTEGER								

VARIABLES	SN	TYPE	RELOCATION	PC	DATA	REAL	ARRAY	SOLV
3415	1	INTEGER				REAL	ARRAY	
3148	2	INTEGER	VECTOR			REAL	ARRAY	
3354	3	INTEGER				REAL	ARRAY	
374	4	REAL				REAL	ARRAY	
520	5	REAL				REAL	ARRAY	
32	6	REAL				REAL	ARRAY	
34	7	REAL				REAL	ARRAY	
36	8	REAL				REAL	ARRAY	
40	9	REAL				REAL	ARRAY	
22	10	REAL				REAL	ARRAY	
24	11	REAL				REAL	ARRAY	
26	12	REAL				REAL	ARRAY	
30	13	REAL				REAL	ARRAY	
3171	14	REAL				REAL	ARRAY	
3172	15	REAL				REAL	ARRAY	
644	16	REAL				REAL	ARRAY	
3448	17	REAL				REAL	ARRAY	
25	18	REAL				REAL	ARRAY	
16	19	REAL				REAL	ARRAY	
20	20	REAL				REAL	ARRAY	
22	21	REAL				REAL	ARRAY	
24	22	REAL				REAL	ARRAY	
3176	23	REAL				REAL	ARRAY	
0	24	REAL				REAL	ARRAY	
0	25	REAL				REAL	ARRAY	
3362	26	REAL				REAL	ARRAY	
0	27	REAL				REAL	ARRAY	
0	28	REAL				REAL	ARRAY	
12	29	REAL				REAL	ARRAY	
14	30	REAL				REAL	ARRAY	
1	31	REAL				REAL	ARRAY	
3	32	REAL				REAL	ARRAY	
5	33	REAL				REAL	ARRAY	
7	34	REAL				REAL	ARRAY	
111	35	REAL				REAL	ARRAY	
3422	36	REAL				REAL	ARRAY	
3423	37	REAL				REAL	ARRAY	
3434	38	REAL				REAL	ARRAY	
3437	39	REAL				REAL	ARRAY	
3356	40	REAL				REAL	ARRAY	
0	41	REAL				REAL	ARRAY	
3324	42	REAL				REAL	ARRAY	
1	43	REAL				REAL	ARRAY	
3	44	REAL				REAL	ARRAY	
5	45	REAL				REAL	ARRAY	
3316	46	REAL				REAL	ARRAY	
7	47	REAL				REAL	ARRAY	
3320	48	REAL				REAL	ARRAY	
3323	49	REAL				REAL	ARRAY	
3322	50	REAL				REAL	ARRAY	
75	51	REAL				REAL	ARRAY	
3420	52	REAL				REAL	ARRAY	
77	53	REAL				REAL	ARRAY	
101	54	REAL				REAL	ARRAY	
181	55	REAL				REAL	ARRAY	
185	56	REAL				REAL	ARRAY	

COMPUTING VESSEL 74/74 OPT=1

VARIABLES SN TYPE RELOCATION

3616	CN00	REAL	
3376	YAF	REAL	
3377	YAO	REAL	
0	TEMP	REAL	PARA
3360	TLI	REAL	
3402	TPR	REAL	
3401	TPR0	REAL	
770	TSOP	REAL	
10	VRN	REAL	SOLV
3534	VO	REAL	PARA
3241	Y	REAL	PARA
2375	HR	REAL	
2377	YO	REAL	
3211	TEOA	REAL	
3257	TL	REAL	
3202	X1	REAL	
3361	X12	REAL	
3207	X16	REAL	
3334	X1	REAL	
3204	X5	REAL	
3336	X7	REAL	
3206	X9	REAL	SOLV
1278	YELLOW	REAL	
3237	VO	REAL	
3353	V10	REAL	
3344	V1	REAL	
3346	V5	REAL	
3350	V7	REAL	
3352	V9	REAL	
3217	W0	REAL	

FILE NAMES MODE
TAPE6 FMT

INLIM FUNCTIONS TYPE ARGS 1 INTRIN

STATEMENT LABELS

1640	1	INACTIVE	1637	2	INACTIVE	2517	5	FMT
0	11		261	12		251	13	
0	16		0	15		362	16	INACTIVE
367	17		23	18		0	30	
121	21	INACTIVE	123	32		1755	80	
0	31		0	32		0	83	INACTIVE
0	41		1762	35		0	109	INACTIVE
1646	110		0	130		771	131	INACTIVE
724	132		730	133		0	134	INACTIVE
735	135		101	140		0	141	INACTIVE
0	142	INACTIVE	1670	143		0	144	INACTIVE
1703	145		0	144		2004	150	
0	151	INACTIVE	0	152		1773	153	
2564	154	FMT	2002	155		2600	156	FMT
0	157		0	159		0	160	
0	161		103	162		0	163	INACTIVE
2305	164		3040	167		1323	169	INACTIVE
0	172	INACTIVE	2355	173		0	174	
0	175		0	185		0	186	

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74/74 OPT=1

COMMON VESSEL

STATEMENT LABELS

2620 187	FMT	0 188
1340 191		1342 192
0 201		0 200
2662 200	FMT	0 330
2131 112		0 331
0 241		2117 252
2730 256	FMT	3062 301
2664 282	FMT	2643 304
472 1300		446 1305
456 1307		456 1308
475 1312		511 1341
1776 1510		0 1640
527 2317		601 2318
557 2340		667 2341
564 2344		600 2345
651 2350		650 2351
2612 6400	FMT	2501 9910

INACTIVE

FMT

FMT

INACTIVE

INACTIVE

0 190
0 200
0 220
2176 331
2075 350
2777 355
2345 370
2356 1234
450 1306
471 1310
1778 1520
0 1900
555 2330
562 2343
604 2346
621 3300

COMMON BLOCKS LENGTH

000	14
PAR	88
FO	22
PC	210
AC	210
PARA	17
SOLV	710
VECTOR	10
INPUT	34
7	76
NUM	11

STATISTICS

PROGRAM LENGTH	76120	1070
COMMON LENGTH	25720	1402

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11/15/74

FTN 4.1PSP367

74/74 OPT=1

FUNCTION ENTH

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FUNCTION ENTH(A,P,TP)
DIMENSION A(14),P(16),X(14),Y(14)
REAL LMS,LSE
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C M2012,M2013,M2014,M2015,M2016,M2017,M2018,M2019,M2020,
C M2021,M2022,M2023,M2024,M2025,M2026,M2027,M2028,M2029,
C M2030,M2031,M2032,M2033,M2034,M2035,M2036,M2037,M2038,
C M2039,M2040,M2041,M2042,M2043,M2044,M2045,M2046,M2047,
C M2048,M2049,M2050,M2051,M2052,M2053,M2054,M2055,M2056,
C M2057,M2058,M2059,M2060,M2061,M2062,M2063,M2064,M2065,
C M2066,M2067,M2068,M2069,M2070,M2071,M2072,M2073,M2074,
C M2075,M2076,M2077,M2078,M2079,M2080,M2081,M2082,M2083,
C M2084,M2085,M2086,M2087,M2088,M2089,M2090,M2091,M2092,
C M2093,M2094,M2095,M2096,M2097,M2098,M2099,M2100,M2101,
C M2102,M2103,M2104,M2105,M2106,M2107,M2108,M2109,M2110,
C M2111,M2112,M2113,M2114,M2115,M2116,M2117,M2118,M2119,
C M2120,M2121,M2122,M2123,M2124,M2125,M2126,M2127,M2128,
C M2129,M2130,M2131,M2132,M2133,M2134,M2135,M2136,M2137,
C M2138,M2139,M2140,M2141,M2142,M2143,M2144,M2145,M2146,
C M2147,M2148,M2149,M2150,M2151,M2152,M2153,M2154,M2155,
C M2156,M2157,M2158,M2159,M2160,M2161,M2162,M2163,M2164,
C M2165,M2166,M2167,M2168,M2169,M2170,M2171,M2172,M2173,
C M2174,M2175,M2176,M2177,M2178,M2179,M2180,M2181,M2182,
C M2183,M2184,M2185,M2186,M2187,M2188,M2189,M2190,M2191,
C M2192,M2193,M2194,M2195,M2196,M2197,M2198,M2199,M2200,
C M2201,M2202,M2203,M2204,M2205,M2206,M2207,M2208,M2209,
C M2210,M2211,M2212,M2213,M2214,M2215,M2216,M2217,M2218,
C M2219,M2220,M2221,M2222,M2223,M2224,M2225,M2226,M2227,
C M2228,M2229,M2230,M2231,M2232,M2233,M2234,M2235,M2236,
C M2237,M2238,M2239,M2240,M2241,M2242,M2243,M2244,M2245,
C M2246,M2247,M2248,M2249,M2250,M2251,M2252,M2253,M2254,
C M2255,M2256,M2257,M2258,M2259,M2260,M2261,M2262,M2263,
C M2264,M2265,M2266,M2267,M2268,M2269,M2270,M2271,M2272,
C M2273,M2274,M2275,M2276,M2277,M2278,M2279,M2280,M2281,
C M2282,M2283,M2284,M2285,M2286,M2287,M2288,M2289,M2290,
C M2291,M2292,M2293,M2294,M2295,M2296,M2297,M2298,M2299,
C M2300,M2301,M2302,M2303,M2304,M2305,M2306,M2307,M2308,
C M2309,M2310,M2311,M2312,M2313,M2314,M2315,M2316,M2317,
C M2318,M2319,M2320,M2321,M2322,M2323,M2324,M2325,M2326,
C M2327,M2328,M2329,M2330,M2331,M2332,M2333,M2334,M2335,
C M2336,M2337,M2338,M2339,M2340,M2341,M2342,M2343,M2344,
C M2345,M2346,M2347,M2348,M2349,M2350,M2351,M2352,M2353,
C M2354,M2355,M2356,M2357,M2358,M2359,M2360,M2361,M2362,
C M2363,M2364,M2365,M2366,M2367,M2368,M2369,M2370,M2371,
C M2372,M2373,M2374,M2375,M2376,M2377,M2378,M2379,M2380,
C M2381,M2382,M2383,M2384,M2385,M2386,M2387,M2388,M2389,
C M2390,M2391,M2392,M2393,M2394,M2395,M2396,M2397,M2398,
C M2399,M2400,M2401,M2402,M2403,M2404,M2405,M2406,M2407,
C M2408,M2409,M2410,M2411,M2412,M2413,M2414,M2415,M2416,
C M2417,M2418,M2419,M2420,M2421,M2422,M2423,M2424,M2425,
C M2426,M2427,M2428,M2429,M2430,M2431,M2432,M2433,M2434,
C M2435,M2436,M2437,M2438,M2439,M2440,M2441,M2442,M2443,
C M2444,M2445,M2446,M2447,M2448,M2449,M2450,M2451,M2452,
C M2453,M2454,M2455,M2456,M2457,M2458,M2459,M2460,M2461,
C M2462,M2463,M2464,M2465,M2466,M2467,M2468,M2469,M2470,
C M2471,M2472,M2473,M2474,M2475,M2476,M2477,M2478,M2479,
C M248
```

C

SYMBOLIC REFERENCE MAP (R=1)

ENTRY POINTS
4 ENTH

VARIABLES	SN	TYPE	RELOCATION	F.P.
0 A		REAL	ARRAY	
113 ANEQ		REAL		Z
74 ANEATL		REAL		Z
46 AN12		REAL		Z
47 AN3M		REAL		Z
50 AN4M		REAL		Z
52 AN65		REAL		Z
60 AN8		REAL		Z
30 CP11		REAL		Z
32 CP13		REAL		Z
26 CP0		REAL		Z
126 PLT		REAL		Z
132 FNTING		REAL		Z
71 F10		REAL		Z
55 F35		REAL		Z
56 F45		REAL		Z
65 F55		REAL		Z
67 F7		REAL		Z
130 F		REAL		Z
110 FMAX		REAL		Z
131 J		INTEGER		
125 LKSE		REAL		
0 M+01		REAL		Z
12 M+011		REAL		Z
14 M+013		REAL		Z
1 M+02		REAL		Z
3 M+04		REAL		Z
5 M+06		REAL		Z
7 M+08		REAL		Z
111 M		REAL		Z
75 SA		REAL		Z
77 SC		REAL		Z
101 SE		REAL		Z
103 SH		REAL		Z
105 SJ		REAL		Z
0 TP		REAL		Z
127 VTA		REAL		Z
137 V		REAL	ARRAY	

INLINE FUNCTIONS TYPE
FLOAT REAL 1 INTDIN

STATEMENT LABELS

101 1 100 2

COMMON BLOCKS LENGTH
76

STATISTICS

PROGRAM LENGTH 1730 123
COMMON LENGTH 1140 76

112 ANA	REAL			
73 ANNA	REAL			Z
61 AN10	REAL			Z
53 AN35	REAL			Z
54 AN45	REAL			Z
51 AN55	REAL			Z
57 AN7	REAL			Z
16 CP	REAL	ARRAY		Z
31 CP12	REAL			Z
33 CP14	REAL			Z
34 DM	REAL	ARRAY		Z
123 ENTH	REAL			
133 ENTH2	REAL			
62 E21	REAL			Z
63 E3M	REAL			Z
64 E4M	REAL			Z
66 E5	REAL			Z
70 E8	REAL			Z
72 FD	REAL			Z
125 I	INTEGER			
124 LBS	REAL	ARRAY		F.P.
0 P	REAL			Z
11 M+010	REAL			Z
13 M+012	REAL			Z
15 M+014	REAL			Z
2 M+03	REAL			Z
4 M+05	REAL			Z
6 M+07	REAL			Z
10 M+09	REAL			Z
106 M7	REAL			Z
76 S0	REAL			Z
100 S0	REAL			Z
102 S6	REAL			Z
104 S1	REAL			Z
106 Y	REAL			Z
107 TR	REAL			Z
109 YTH	REAL	ARRAY		
134 YTH	REAL			
155 Y	REAL			

66 3

.6421300E+00	.1727301E+02	.3467153E+02	.5819492E+02	0.
.1731727E+01	.6565214E+01	0.	.7070775E+02	0.
.0011410E+00	.2670702E+00	.4153075E+01	.3768770E+01	.4003573E+02
.1017064E+01	.3007001E+02	.9023072E+02	0.	.4062052E+16
0.	0.	0.	0.	0.
.1521340E+15	.1777700E+15	.1915970E+05	.1040993E+02	.1000014E+02
.1350765E+00	.0060577E+03	.2070767E+02	.3000715E+02	0.
.0670615E+02	.1020470E+01	0.	.6233100E+02	.2900715E+02
.1900651E+10	.3051703E+12	.8265915E+05	.6509232E+02	.4293203E+02
.1857100E+01	.4057060E+02	.1215015E+01	0.	.1572906E+19
0.	0.	0.	0.	0.
.6401000E+29	.9014431E+21	.1200150E+01	.1013670E+03	.1011337E+02
.4310766E+02	.1111720E+02	.361214E+02	.3071310E+02	0.
.0607000E+02	.1057657E+01	0.	.6211761E+02	0.
.1000651E+10	.3051703E+12	.8265915E+05	.6509232E+02	.4290994E+02
.1857100E+01	.4057060E+02	.1215015E+01	0.	.1572906E+19
0.	0.	0.	0.	0.
.5776627E+10	.1050602E+10	.2297007E+01	.7763093E+04	.7990007E+01
.3615427E+00	.0506937E+03	.2570211E+02	.3035607E+02	0.
.7220000E+02	.1667560E+00	0.	.5366277E+02	0.
.1074065E+13	.3017770E+15	.0500002E+01	.2010072E+03	.2062424E+02
.1244557E+01	.3106700E+02	.0557365E+02	0.	.3003130E+23
0.	0.	0.	0.	0.
.1000000E+26	.1210265E+26	.7267074E+02	.4503500E+05	.0004017E+01
.3600011E+00	.1961650E+02	.3126051E+02	.3033115E+02	0.
.7231605E+02	.1516077E+00	0.	.5301430E+02	0.
.1074065E+13	.3017770E+15	.0500002E+01	.2010072E+03	.2062940E+02
.1244557E+01	.3106700E+02	.0557365E+02	0.	.3003130E+23
0.	0.	0.	0.	0.

1. 1. 1.2 1.2 1.5

NOT IN PROPORTIONS---DEVELOPED ON 7-21-72

1000.

1000.

900.

10000.

1763.

500.

0.

0.

0.

0.

0.

0.

0.

0.

0.

0.

0.

0.

0.

0.

0.

0.

NOTED

Year	1972	1973	1974	1975	1976	1977	1978	1979	1980	1981	1982	1983	1984	1985	1986	1987	1988	1989	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032	2033	2034	2035	2036	2037	2038	2039	2040	2041	2042	2043	2044	2045	2046	2047	2048	2049	2050	2051	2052	2053	2054	2055	2056	2057	2058	2059	2060	2061	2062	2063	2064	2065	2066	2067	2068	2069	2070	2071	2072	2073	2074	2075	2076	2077	2078	2079	2080	2081	2082	2083	2084	2085	2086	2087	2088	2089	2090	2091	2092	2093	2094	2095	2096	2097	2098	2099	2100
1972	1973	1974	1975	1976	1977	1978	1979	1980	1981	1982	1983	1984	1985	1986	1987	1988	1989	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032	2033	2034	2035	2036	2037	2038	2039	2040	2041	2042	2043	2044	2045	2046	2047	2048	2049	2050	2051	2052	2053	2054	2055	2056	2057	2058	2059	2060	2061	2062	2063	2064	2065	2066	2067	2068	2069	2070	2071	2072	2073	2074	2075	2076	2077	2078	2079	2080	2081	2082	2083	2084	2085	2086	2087	2088	2089	2090	2091	2092	2093	2094	2095	2096	2097	2098	2099	2100	

007-601 00000'S 0.0001' 00000' 00000'

M0031 KFO JF M

5-10-63 - 611041138

	F70	F69	F75	F68	F67	E6	E10
.....	\$300-	\$440	\$175	\$555	\$545	\$0	\$10
" "	2600-	2700	22000-	10000-	5500.	7000.	1.

CONTACT DATA:

A	B	C	D	E	F	G	H	I	J
255147	255147	1.40	1.50	1.00	7.00	0.00		1.516000	0.00

545 LA² CONSTANT = 86

ИЗДАТЕЛЬСТВО «НАУКА» 1980

$$\begin{aligned} \text{WACC} &= \text{V.L. COEFF.} \times \text{COST OF DEBT} + (1 - \text{V.L. COEFF.}) \times \text{COST OF EQUITY} \\ &= 27.5\% \times 5.00\% + (1 - 27.5\%) \times 12.00\% = 9.38\% \end{aligned}$$
[illegible]

667 = 1631019999 1652410

5311836536 0012ans

Conc'n of Catalyst	wt.-%	Density	wt. cap.	Reaction	ml. of 1393M.
1	117.9	.64	70.00	1	1393M.
2	137.0	.65	73.60	2	1312M.
3	105.0	.64	70.00	3	1375M.
4	122.5	.66	73.90	4	999M.
5	227.0	.68	70.00	5	1176M.
6	227.0	.65	73.00	6	1452M.
7	213.0	.64	70.00	7	2376M.
8	252.0	.68	71.00	8	3218M.
9	87.9	1.01	1.01	9	1320M.
10	92.0	.65	15.00	10	0

STAGE 1
NITRATION 1A
VOL. = 52.1
TEMP. = 51.0
NITRATION 1B
VOL. = 52.1
TEMP. = 51.0

SEPARATION 1
VOL. = 29.1
NATURAL SETTING = 1
ENTRAPMENT
ORGANIC IN ACID .00071
ACID IN ORGANIC .00000

STAGE 2
NITRATION 2
VOL. = 50.1
TEMP. = 64.0

SEPARATION 2
VOL. = 29.1
NATURAL SETTING = 1
ENTRAPMENT
ORGANIC IN ACID .00007
ACID IN ORGANIC .00015

STAGE 3
NITRATION 3A
VOL. = 51.5
TEMP. = 61.0
NITRATION 3B
VOL. = 52.1
TEMP. = 65.0

SEPARATION 3
VOL. = 28.1
NATURAL SETTING = 0
ENTRAPMENT
ORGANIC IN ACID .00032
ACID IN ORGANIC .00018

STAGE 4
NITRATION 4
VOL. = 51.5
TEMP. = 60.0

SEPARATION 4
VOL. = 29.1
NATURAL SETTING = 5
ENTRAPMENT
ORGANIC IN ACID .00047
ACID IN ORGANIC .00021

STAGE 5
NITRATION 5
VOL. = 49.2
TEMP. = 60.0

SEPARATION 5
VOL. = 29.1
NATURAL SETTING = 2
ENTRAPMENT
ORGANIC IN ACID .00111
ACID IN ORGANIC .00050

STAGE 6

Shillington, Virginia

[illegible]

	AMNT	MMNT	AMNT	MMNT	ATMT	MMNT	ATMT	MMNT	TMP	TMBA	MMO3	YOL	M2S04	MMO504	M2O	S03
ACID PHASE	.000	.000	.025	.000	10.781	.461	.000	.000	.000	.000	75.350	0.000	71.522	.151	0.000	53.927
ORG. PHASE	.000	.000	.072	.000	30.277	1.303	.000	.000	.000	.001	0.000	.000				

CFEADATOR 6 TEMPERATURE = 110.2

	AMNT	MMNT	AMNT	MMNT	ATMT	MMNT	ATMT	MMNT	TMP	TMBA	MMO3	YOL	M2S04	MMO504	M2O	S03
ACID PHASE	.000	.000	.072	.000	10.781	.460	.000	.000	.000	.000	75.330	0.000	71.547	.155	0.000	53.927
ORG. PHASE	.000	.000	.072	.000	30.280	1.303	.000	.000	.000	.001	0.000	.000				

GAS DATA

VESSEL	FOR	MOX	TIME	C ₂	O
1	.0000	.0000	.0000	.0000	.0047134
2	.0000	.0000	.0000	.0000	.0017639
3	.0000	.0000	.0000	.0000	.0016771
4	.1504	.0571	.0010	.0000	.4809113
5	.0011	.0201	.0005	.0000	.4777625
6	1.2100	1.3364	.0135	.0000	.9999992
7	2.0000	1.0717	.0136	.0000	.9999996
8	.7654	.2534	.0032	.0000	.9999997
9	1.4701	.5201	.0062	.0000	.9999998
10	.2430	.0000	.0011	.0000	.9999998
11	.5000	.1032	.0020	.0000	.9999999
12	.0534	.0103	.0007	.0000	.9999999
13	.1702	.0014	.0025	.0000	1.0000000
14	.0001	.0022	.0000	.0000	1.0000000
TOTAL	10.1130	3.6305	.0460	.0000	

VESSEL TIME CONSTANTS AND VOLUMETRIC FLOWS

VESSEL	QA	QP	QI	TAU	FO
1	107.34	65.70	202.73	.2570	.2732
2	107.34	65.77	206.11	.2634	.2685
3	107.34	65.77	206.11	.2685	.2650
4	156.13	125.32	281.45	.1703	.4453
5	156.04	125.35	281.40	.2714	.2450
6	137.75	126.71	262.47	.2834	.4751
7	125.01	126.62	400.23	.1044	.3494
8	122.62	125.35	690.92	.0404	.2450
9	152.15	121.76	673.70	.1124	.2570
10	151.15	122.16	673.31	.1425	.2550
11	140.74	121.60	311.45	.1933	.3907
12	140.57	121.78	311.35	.1866	.2550
13	154.00	79.64	234.49	.2567	.3395
14	154.04	79.64	234.49	.2957	.2550

COMPARISON OF MEASUREMENTS IN THE ACID PHASE

VESSEL	VF04
1	.041023
2	.061037
3	.091037
4	.211020
5	.211020
6	.222070
7	.051020
8	.050000
9	.052023
10	.052023
11	.055015
12	.055007
13	.060036
14	.060037

*****DISPERSED ORGANIC MOL RUPS*****

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	13.74	641.72	222.82	5.21	1.20	.01	.00	.00	.00	.00	.00	.00	.00	.00
2	2.26	21.16	7.45	.17	.94	.00	.00	.00	.00	.00	.00	.00	.00	.00
3	2.68	282.23	71.60	963.66	221.69	669.51	280.95	75.83	66.88	23.91	31.26	6.56	3.37	.01
4	17.51	16.28	5.94	74.50	7.07	15.20	4.01	1.04	.56	.19	.15	.03	.01	.03
5	155.23	126.25	45.66	778.13	177.11	1496.69	1279.82	346.44	1124.57	482.82	2014.04	421.69	1775.84	427.95
6	4.32	6.72	2.37	10.20	9.52	74.53	63.89	17.29	50.70	10.16	87.33	10.28	75.91	18.29
7	2.0	4.0	.20	.00	.00	.01	.01	.00	.01	.00	.02	.00	.02	.00
8	2.0	4.0	.20	.01	.00	.03	.03	.01	.03	.01	.06	.01	.06	.02
9	39.72	21.81	7.65	65.91	18.40	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00
10	.1	.46	.02	.30	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
TOTAL	1076.12	174.15	344.71	1858.70	427.39	2758.97	1628.71	448.04	1282.74	445.11	2133.09	446.59	1055.21	447.89

TOTAL Wt. MP OF DISPERSED CLASS 7 MATERIAL IN MITIGATION SECTION = 13176.23

TOTAL Wt. MP OF DISPERSED TNT IN MITIGATION SECTION = 2964.52

TOTAL Wt. MP OF DISPERSED TNT IN MITIGATION SECTION = 11056.80

*****DISSOLVED ORGANIC MOL RUPS*****

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	12.31	6.24	2.51	.45	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
2	3.37	21	.27	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
3	5.31	1.00	.91	65.14	25.30	81.10	60.44	16.94	27.20	4.84	7.23	.74	1.17	.04
4	2.37	1.16	.27	1.76	.22	1.27	.99	.14	.22	.02	.03	.00	.00	.00
5	2.24	1.23	.50	79.14	24.31	184.27	317.00	155.35	648.55	176.60	465.70	193.28	618.42	226.45
6	2.17	1.27	.83	1.99	1.44	9.67	15.97	7.32	28.76	7.76	29.19	8.20	26.43	9.66
7	2.0	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
8	2.0	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
9	2.0	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
10	2.0	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00	.00
TOTAL	21.44	9.07	3.94	52.00	51.86	276.99	404.62	179.75	508.82	189.30	493.26	202.33	646.05	236.16

TOTAL Wt. MP OF DISSOLVED CLASS 7 MATERIAL IN MITIGATION SECTION = 3281.04

TOTAL Wt. MP OF DISSOLVED TNT IN MITIGATION SECTION = 290.87

TOTAL Wt. MP OF DISSOLVED TNT IN MITIGATION SECTION = 2906.72

TOTAL Wt. MP OF ALL TNT IN MITIGATION SECTION = 3282.59

TOTAL Wt. MP OF ALL TNT IN MITIGATION SECTION = 14053.04

TOTAL Wt. MP OF ALL CLASS 7 MATERIAL IN MITIGATION SECTION = 16447.27

100 = 0.077 76666 = 0.3999

[illegible]

51451° = 603 51452° = 703

[illegible]

$\text{FCI} = -0.50$ $\text{FCI} = 0.03$ $\text{FCI} = 0.03$

[illegible]

STAGE 4 FC8 = -2067 FC9 = .92621

*****ELEMENTAL MATERIAL BALANCES*****

OVERALL MATERIAL BALANCE			
	MOLEC IN	MOLEC OUT	DIFFERENCE
FLUENT			
CARBON	122,552	105,541	-17,011
HYDROGEN	764,617	764,617	-0.000
HYDROGEN	826,850	826,850	-0.000
HYDROGEN	84,104	84,104	-0.000
CHLORINE	105,313	105,313	-0.000
STAGE 1			
FLUENT			
CARBON	229,525	229,525	-0.000
HYDROGEN	641,760	641,760	-0.000
HYDROGEN	757,150	757,150	-0.000
HYDROGEN	84,270	84,270	-0.000
CHLORINE	105,247	105,247	-0.000
STAGE 2			
FLUENT			
CARBON	301,570	301,570	-0.000
HYDROGEN	649,740	649,740	-0.000
HYDROGEN	933,645	933,645	-0.000
HYDROGEN	157,340	157,340	-0.000
CHLORINE	111,440	111,440	-0.000
STAGE 3			
FLUENT			
CARBON	415,700	415,700	-0.000
HYDROGEN	540,470	540,470	-0.000
HYDROGEN	879,270	879,270	-0.000
HYDROGEN	109,240	109,240	-0.000
CHLORINE	115,100	115,100	-0.000
STAGE 4			
FLUENT			
CARBON	365,510	365,510	-0.000
HYDROGEN	419,500	419,500	-0.000
HYDROGEN	772,670	772,670	-0.000
HYDROGEN	171,540	171,540	-0.000
CHLORINE	113,610	113,610	-0.000
STAGE 5			
FLUENT			
CARBON	375,740	375,740	-0.000
HYDROGEN	417,850	417,850	-0.000
HYDROGEN	773,240	773,240	-0.000
HYDROGEN	173,500	173,500	-0.000
CHLORINE	105,410	105,410	-0.000
STAGE 6			
FLUENT			
CARBON	249,710	249,710	-0.000
HYDROGEN	342,700	342,700	-0.000
HYDROGEN	653,430	653,430	-0.000
HYDROGEN	141,700	141,700	-0.000
CHLORINE	105,070	105,070	-0.000
VESSEL 1			
FLUENT			
CARBON	183,270	183,270	-0.000
HYDROGEN	712,440	712,440	-0.000
HYDROGEN	703,110	703,110	-0.000

WESSEL 1	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 2	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 3	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 4	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 5	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 6	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 7	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 8	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 9	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 10	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 11	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 12	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 13	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 14	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 15	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 16	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 17	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 18	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 19	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000
WESSEL 20	WELFC IN	WELFC OUT	DIFFERENCE
FLIGHT	274,215	274,215	0.000
CANADA	274,215	274,215	0.000

VESSEL 10			
ELEMENT	WLF5 IN	WLF5 OUT	DIFFERENCE
CARBON	406.8134	406.8134	.0000
HYDROGEN	805.8291	805.8277	.0014
NIITROGEN	1682.9088	1682.8955	.0025
CLIP-UP	277.8276	277.8276	0.0000
	205.7315	205.7315	.0000
VESSEL 11			
ELEMENT	WLF5 IN	WLF5 OUT	DIFFERENCE
CARBON	621.8061	621.8061	-.0013
HYDROGEN	527.4263	527.4270	.0033
NIITROGEN	1032.6366	1032.6304	.0063
CLIP-UP	216.6271	216.6270	-.0007
	159.6271	159.6269	.0004
VESSEL 12			
ELEMENT	WLF5 IN	WLF5 OUT	DIFFERENCE
CARBON	621.8172	621.8172	.0000
HYDROGEN	527.4270	527.4277	.0003
NIITROGEN	1031.5110	1031.5119	.0005
CLIP-UP	216.6168	216.6168	.0000
	159.6263	159.6263	.0000
VESSEL 13			
ELEMENT	WLF5 IN	WLF5 OUT	DIFFERENCE
CARBON	701.0700	701.0660	-.0176
HYDROGEN	706.2710	706.2711	-.0148
NIITROGEN	783.5921	783.6128	-.0200
CLIP-UP	156.8176	156.8260	-.0046
	125.6266	125.6295	-.0062
VESSEL 14			
ELEMENT	WLF5 IN	WLF5 OUT	DIFFERENCE
CARBON	331.8161	331.8161	.0000
HYDROGEN	706.2711	706.2713	.0000
NIITROGEN	783.5959	783.2959	.0001
CLIP-UP	156.7665	156.7665	.0000
	125.6295	125.6295	.0000

000555000007

YIELD = 80.213 MILE DCL FOR COMPRESSION TO DMI

LINE/NO COMPRESS DCL 25419.46

WT DCL IN IN COMPRESS DCL = .1823

RAW MATERIALS COST: 5419 OF A-TOT = .850040

COMPRESS FLOW: 13665.0063

ACID NO. 13665.0063

WGT. NO. 13665.0063

TOTAL 13665.0063

WT DCL TOTAL NO = .5997

WT DCL DISCLOSED NO = .2826

WT DCL IN DISCLOSED NO = 22.11906

STAGE DATA

STAGE	A-NITRATION	B-NITRATION	ACT NITRIC	ACT SULPHURIC	INT NITRIC	INT SULPHURIC	TOTAL ACTIVITY	NO DENSITY
1	26.711	1.272	2.090	65.440	5.205	70.275	64.691	73.849
2	22.954	.797	1.123	76.571	19.795	82.287	86.972	87.692
3	14.142	.793	17.404	80.430	16.890	86.717	93.340	90.076
4	3.727	.276	12.900	98.397	16.818	92.155	101.385	90.603
5	1.175	.015	12.940	93.473	13.253	93.999	103.736	90.771
6	.506	.003	12.133	95.037	12.407	95.135	106.672	90.759

NITRATION UNIT OUTPUT

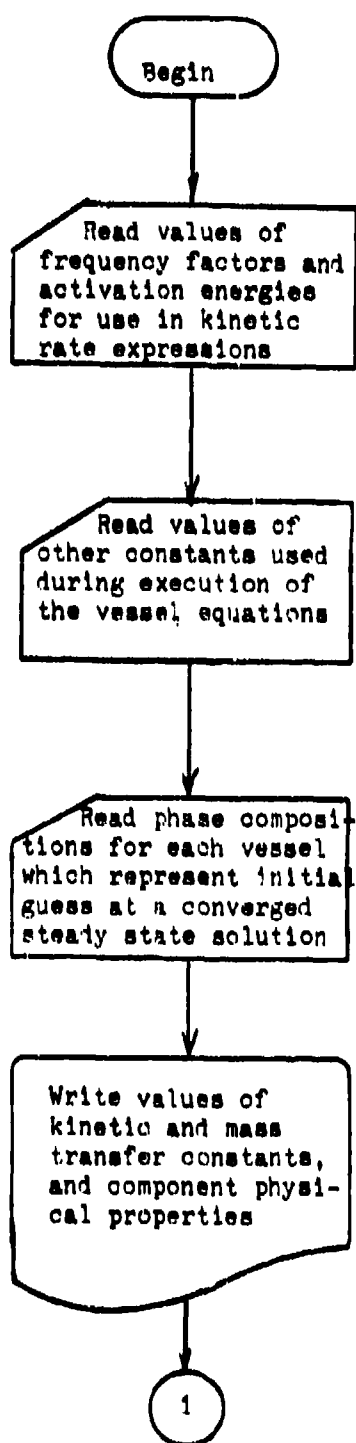
NITRATION	BTU
1	165114.7
2	200236.1
3	200404.1
4	154121.6
5	126690.7
6	97633.0
7	41761.1
8	-13927.8

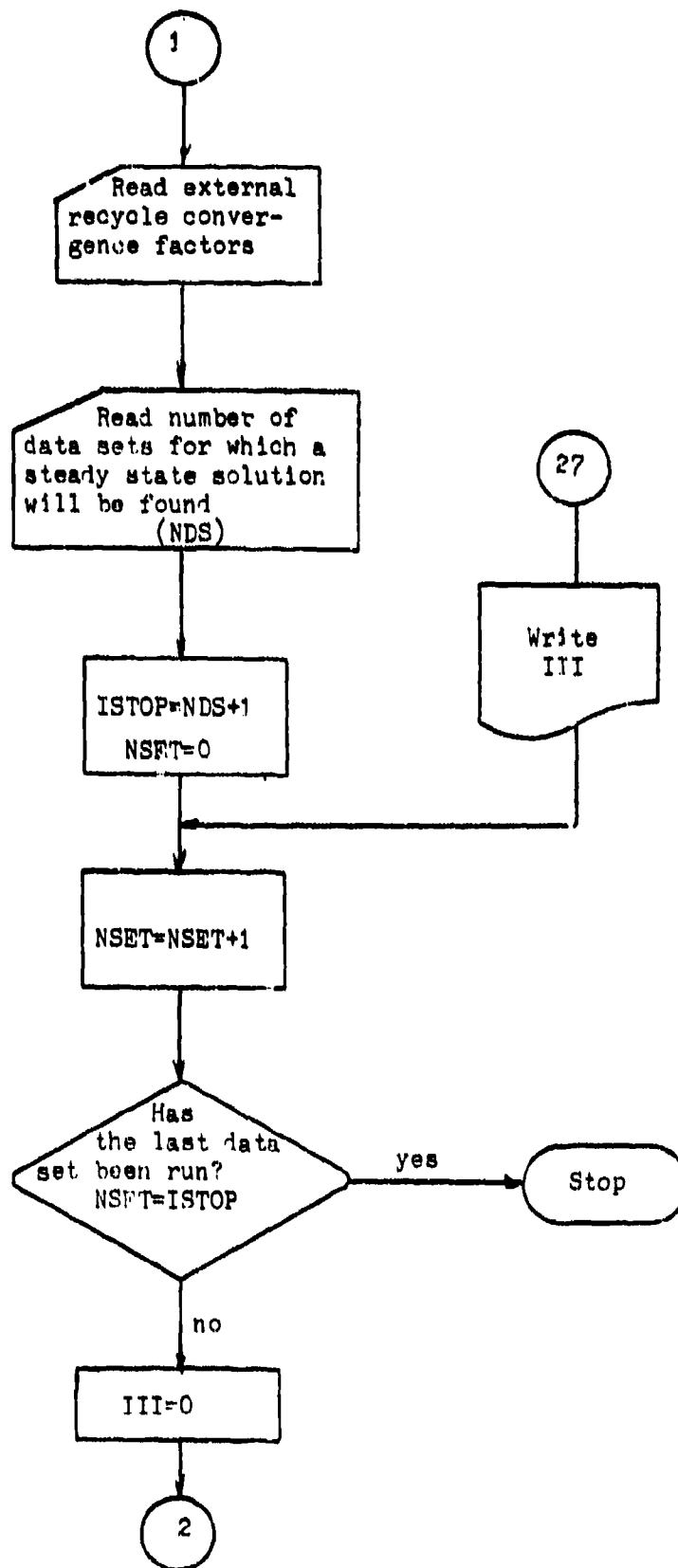
NUMBER OF VESSEL EMULATION ITERATIONS FOR THIS DATA SET 6238

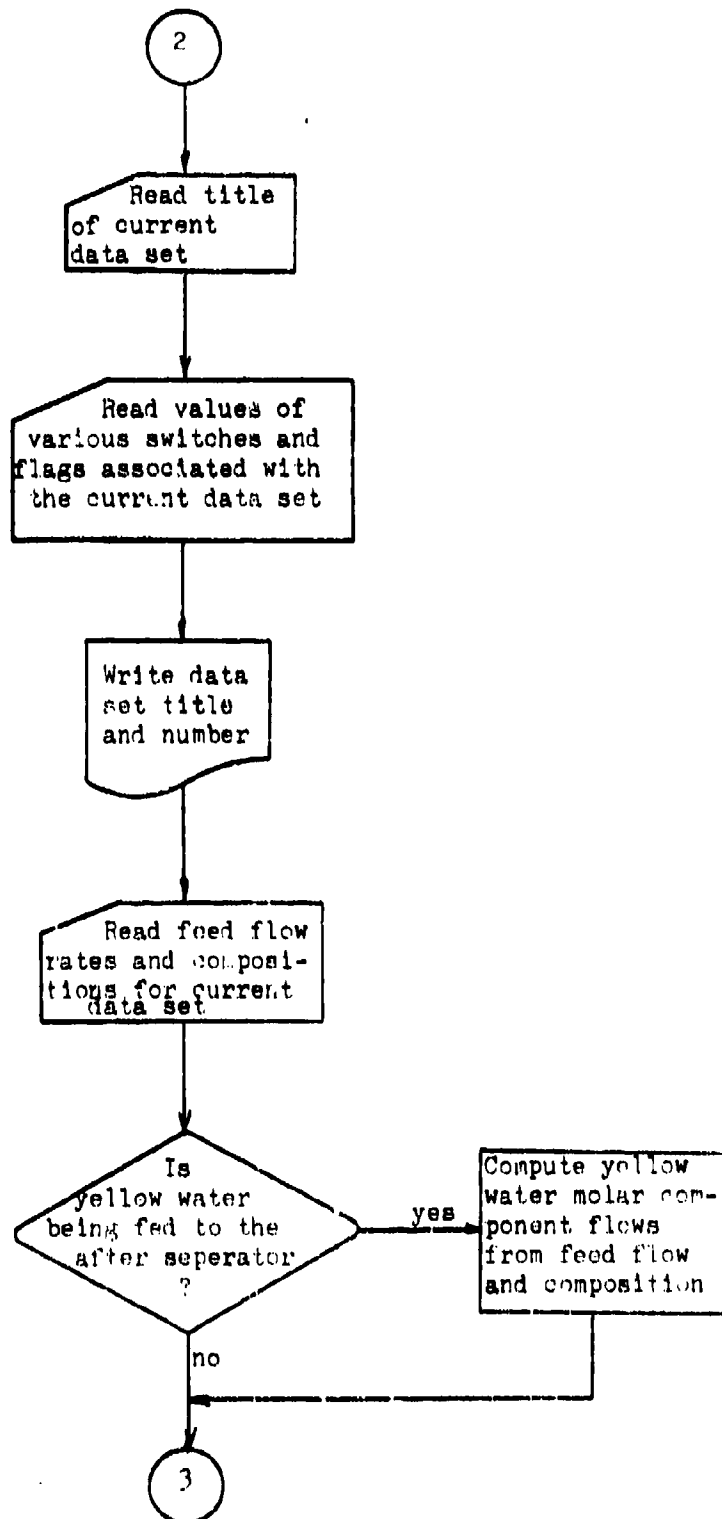
APPENDIX G

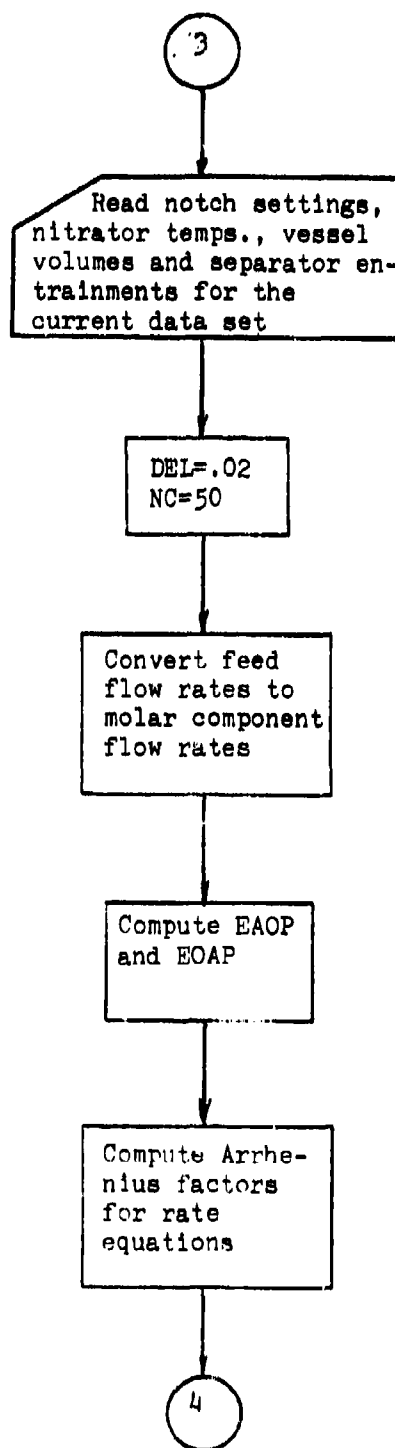
Steady State Simulation--Program Flowchart

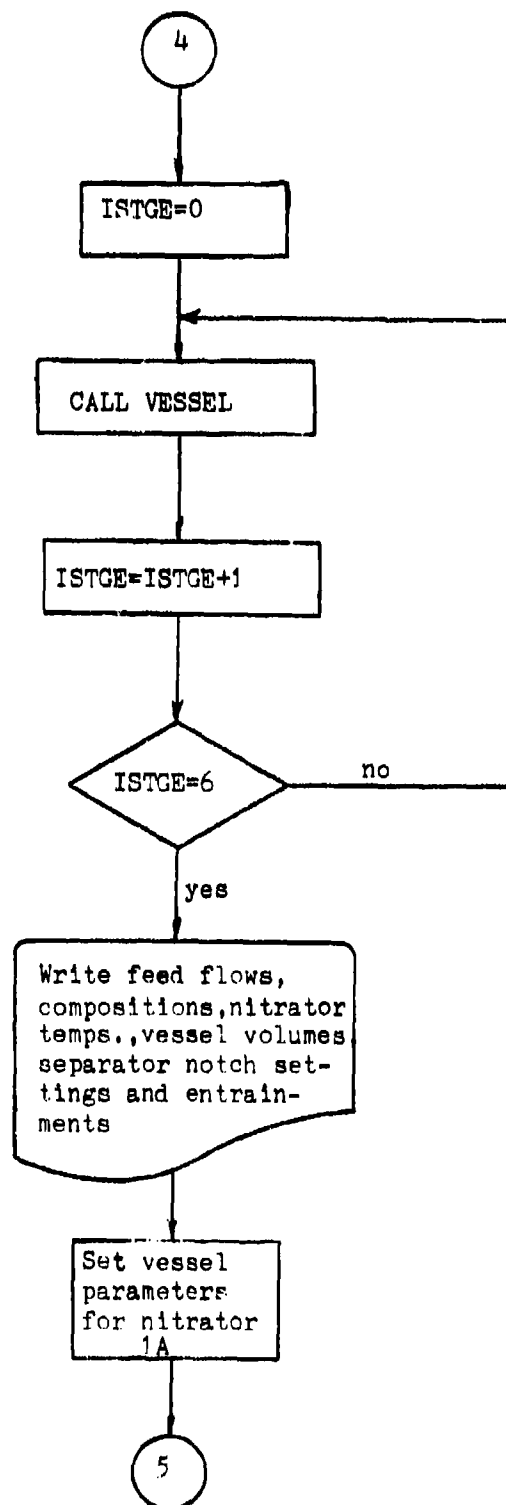
Main Program

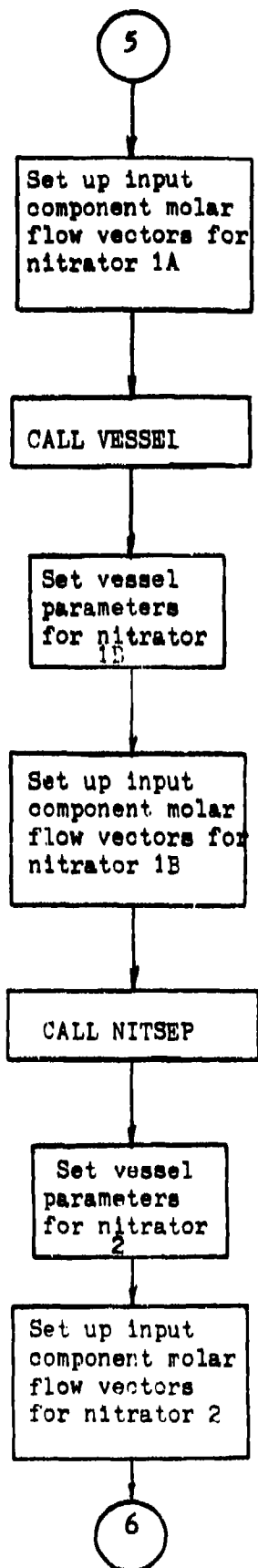


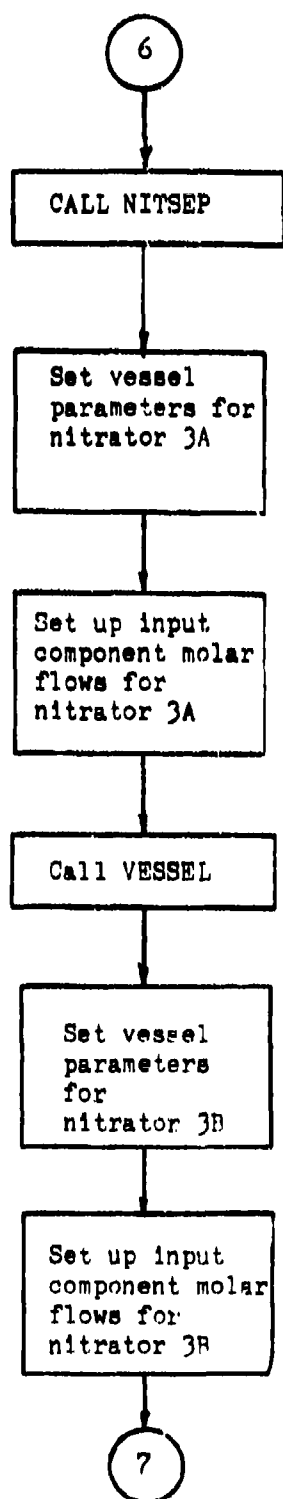


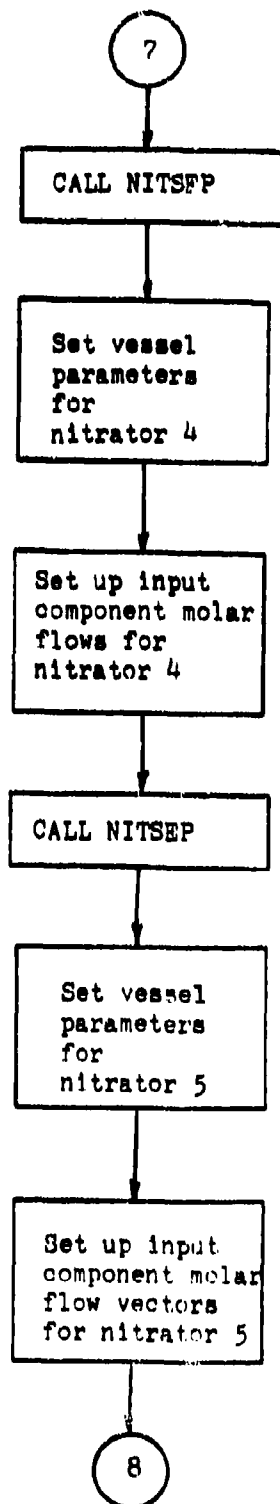


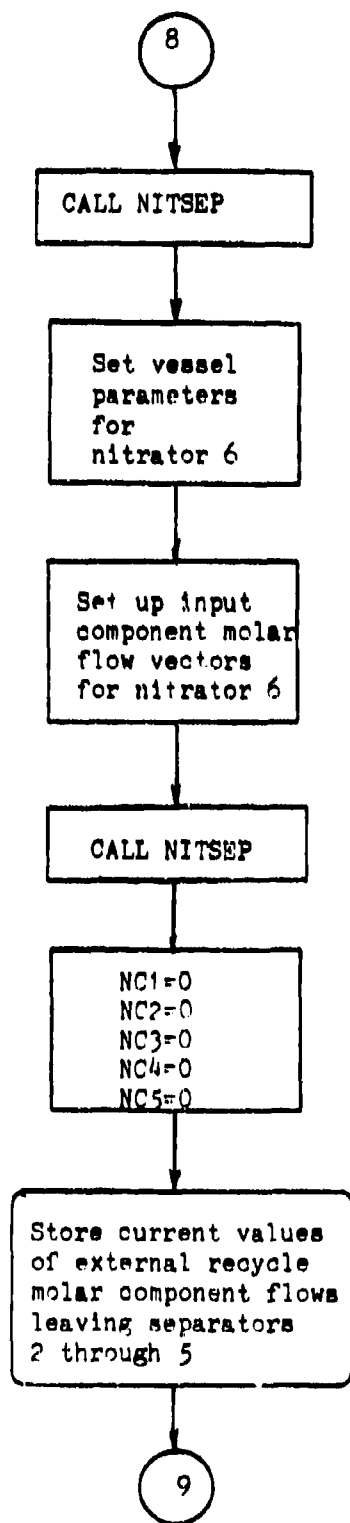


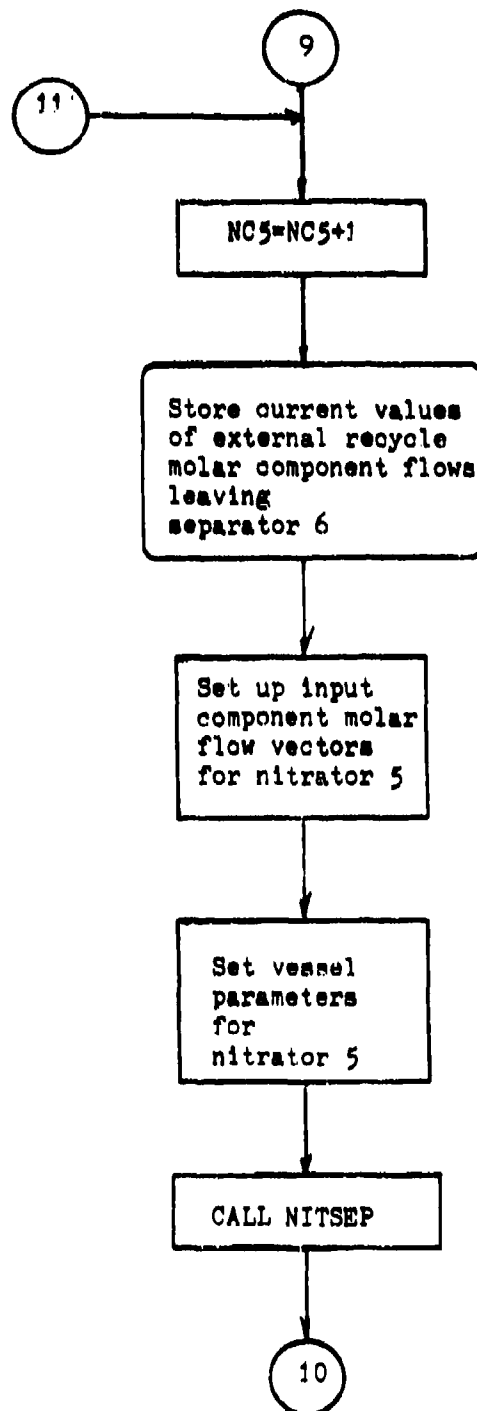


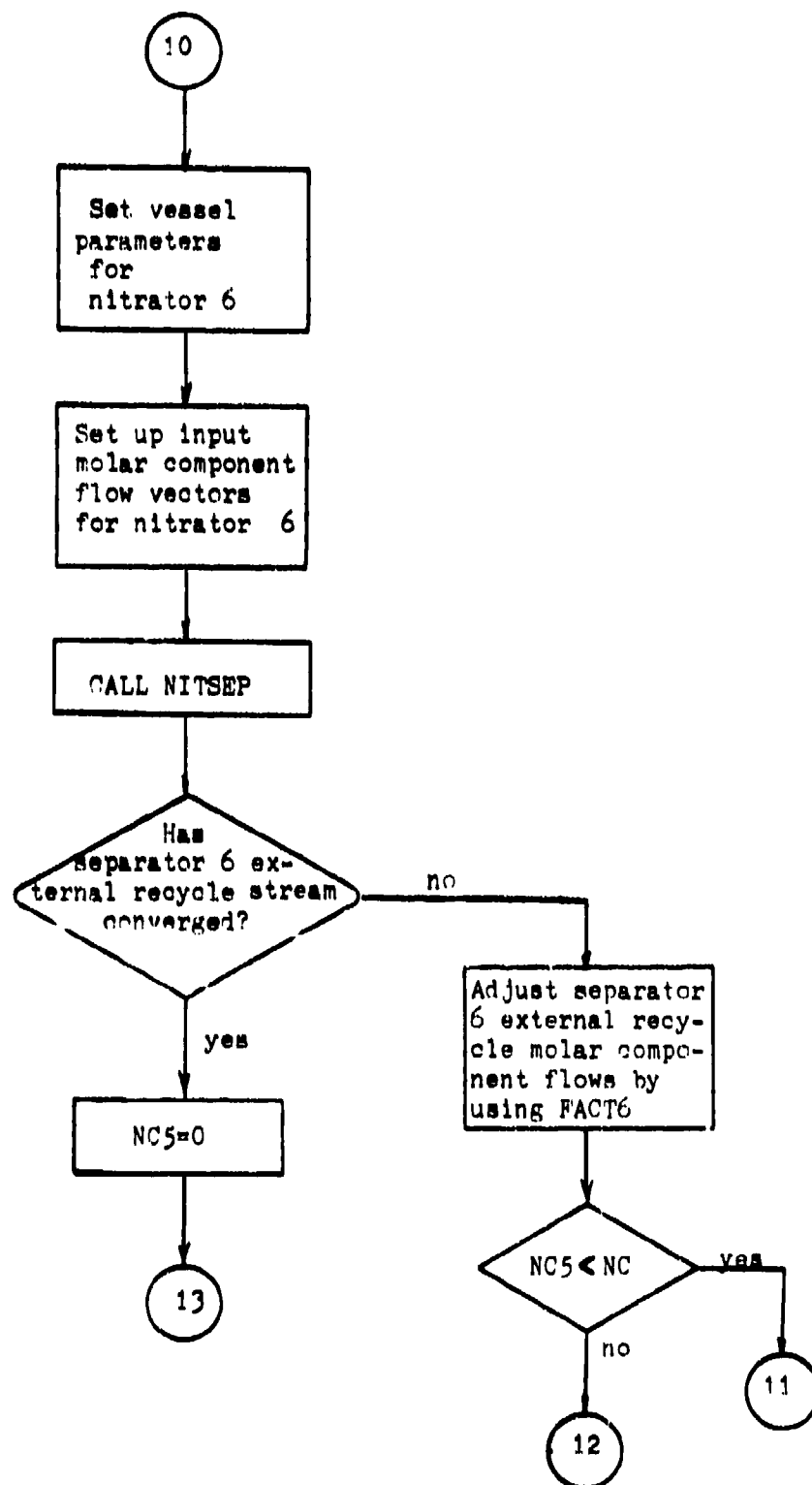








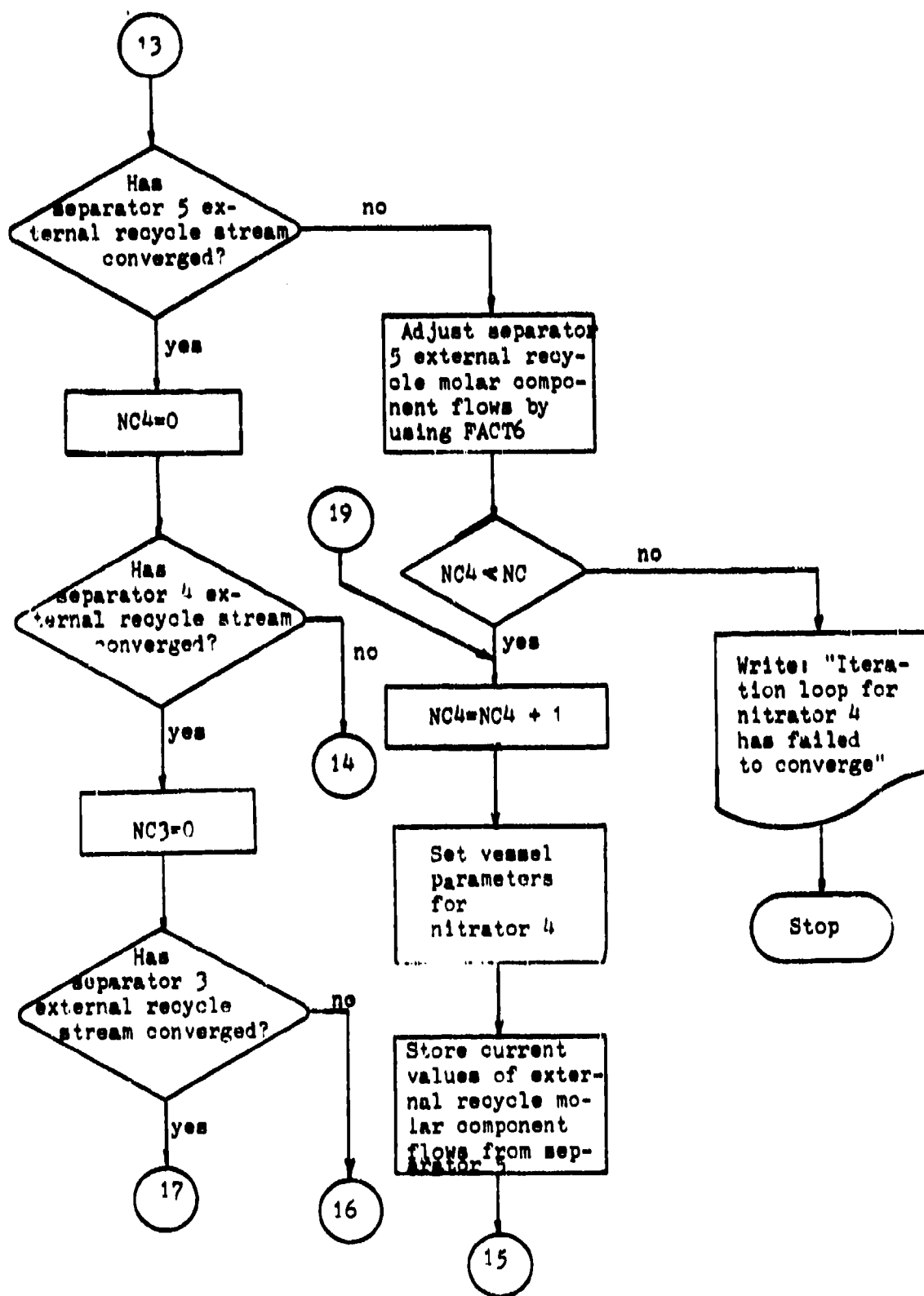


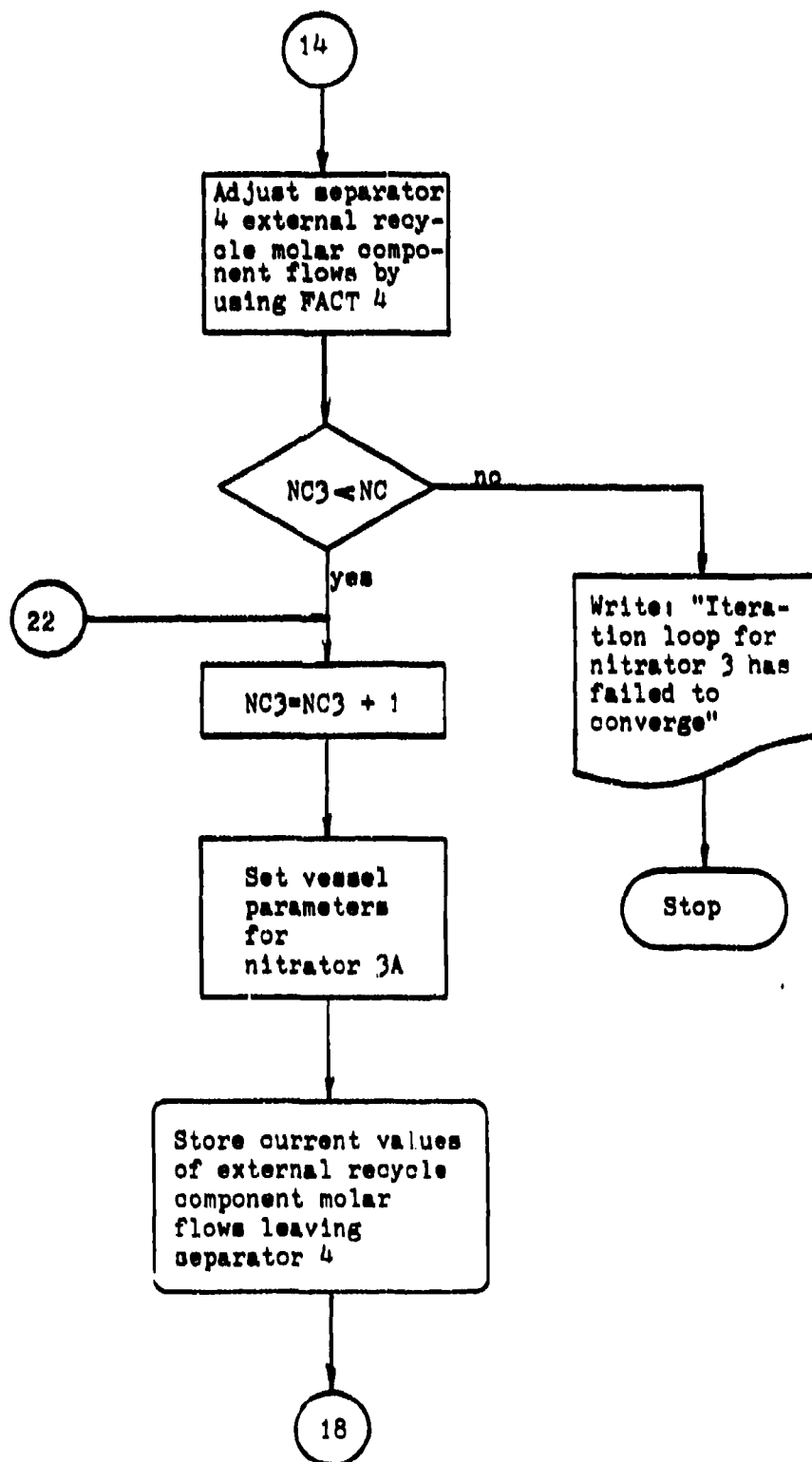


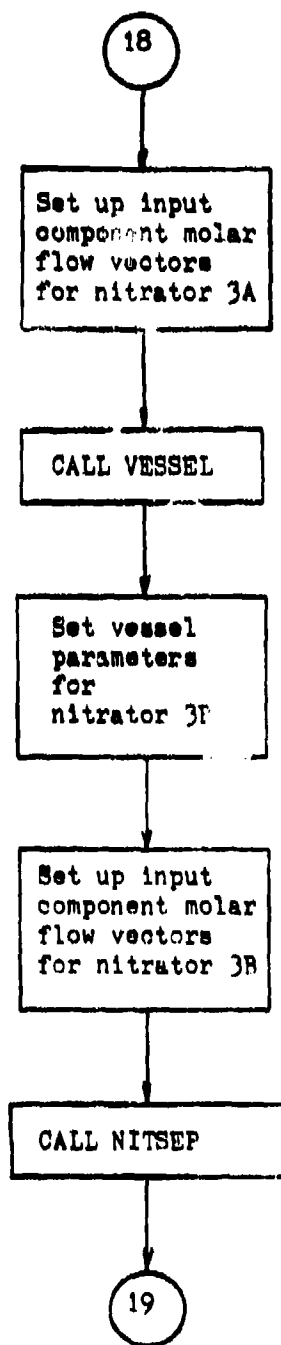
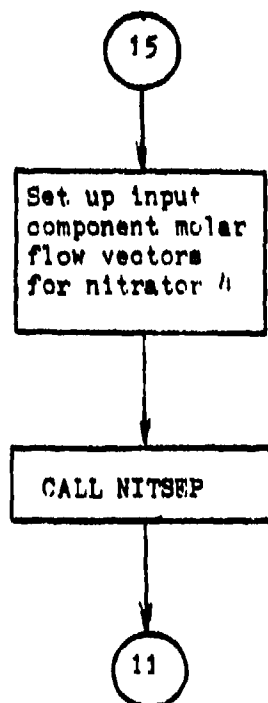
12'

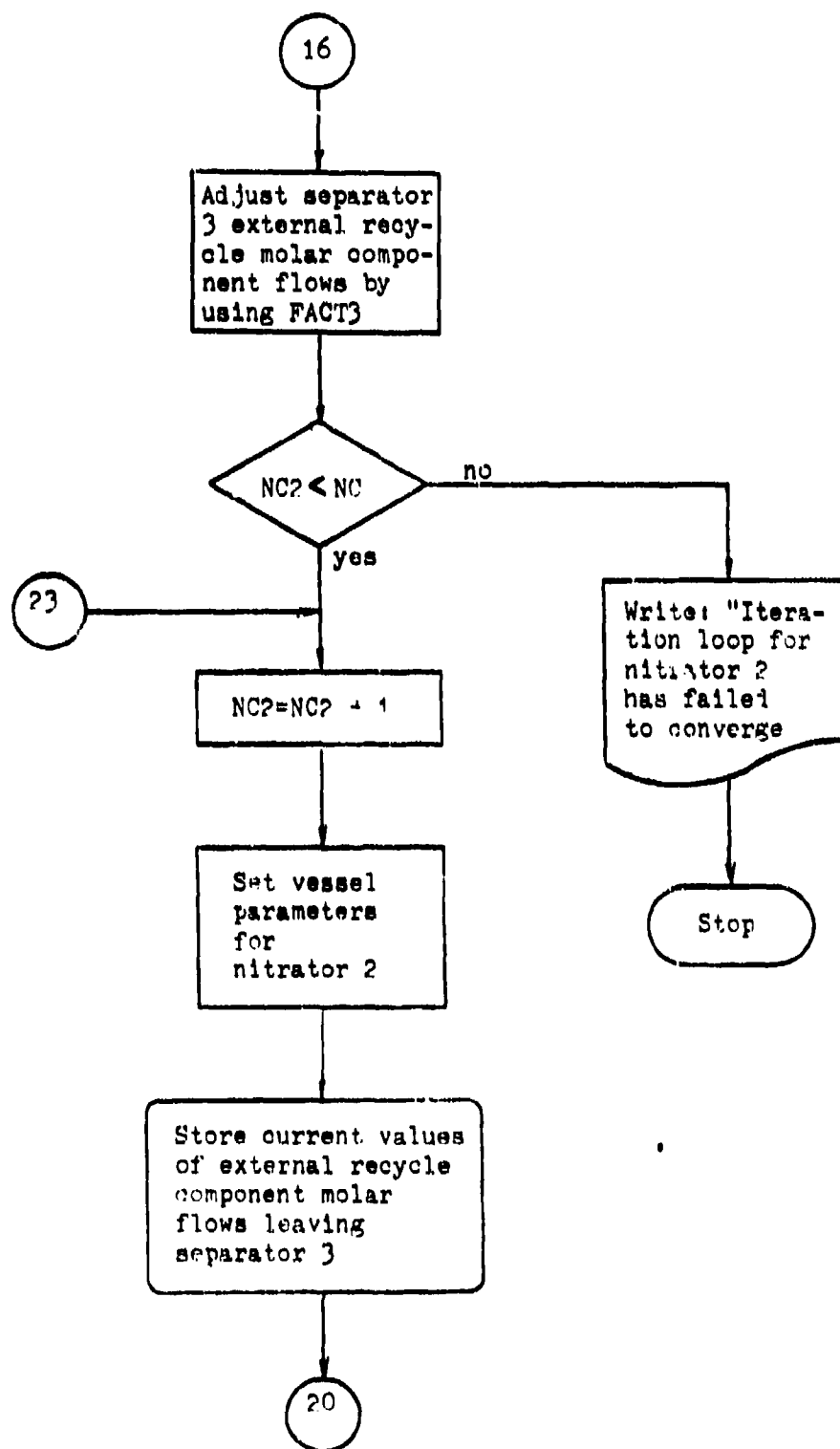
Write: "Iteration loop
for nitrater
5 failed to
converge"

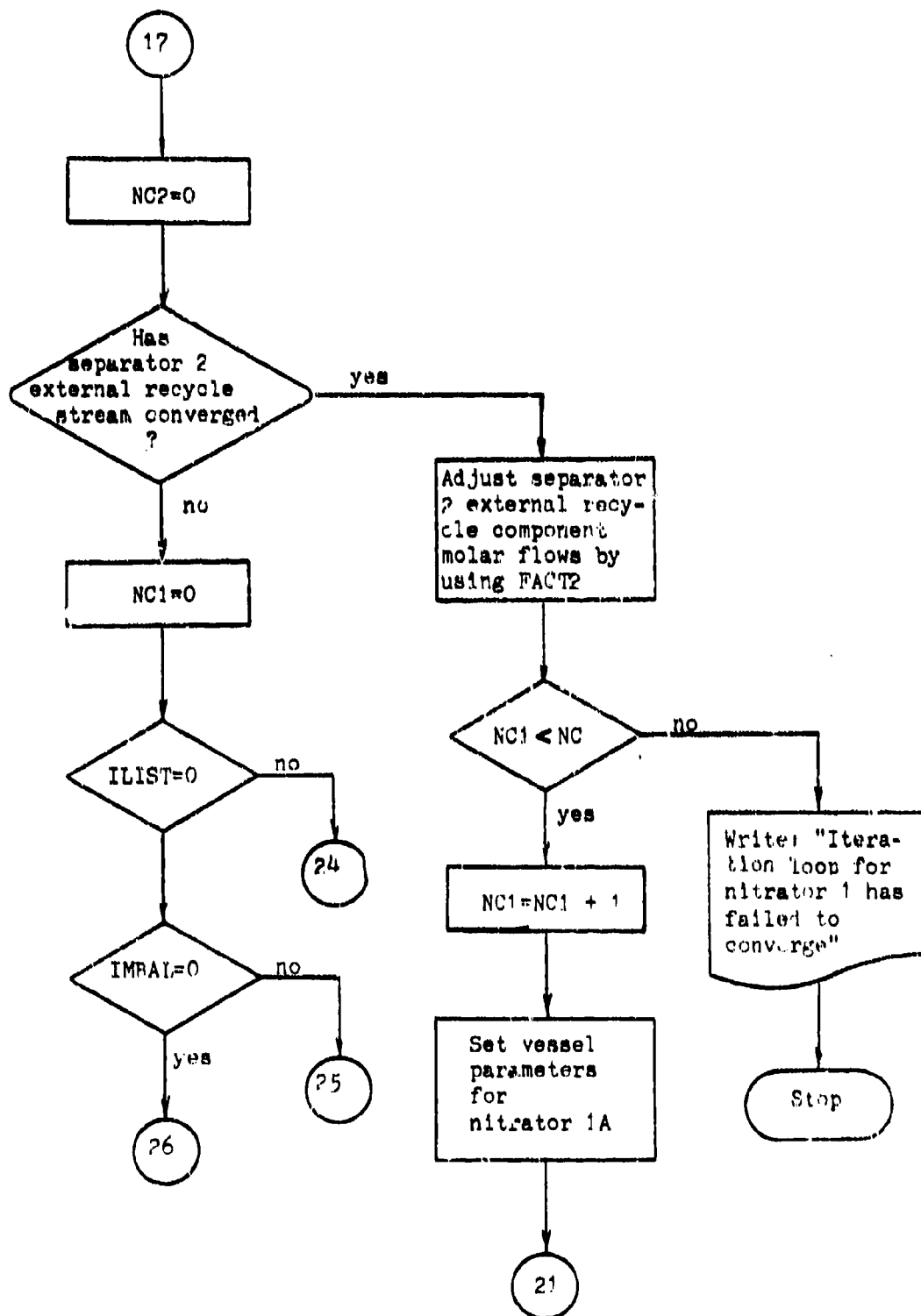
Stop

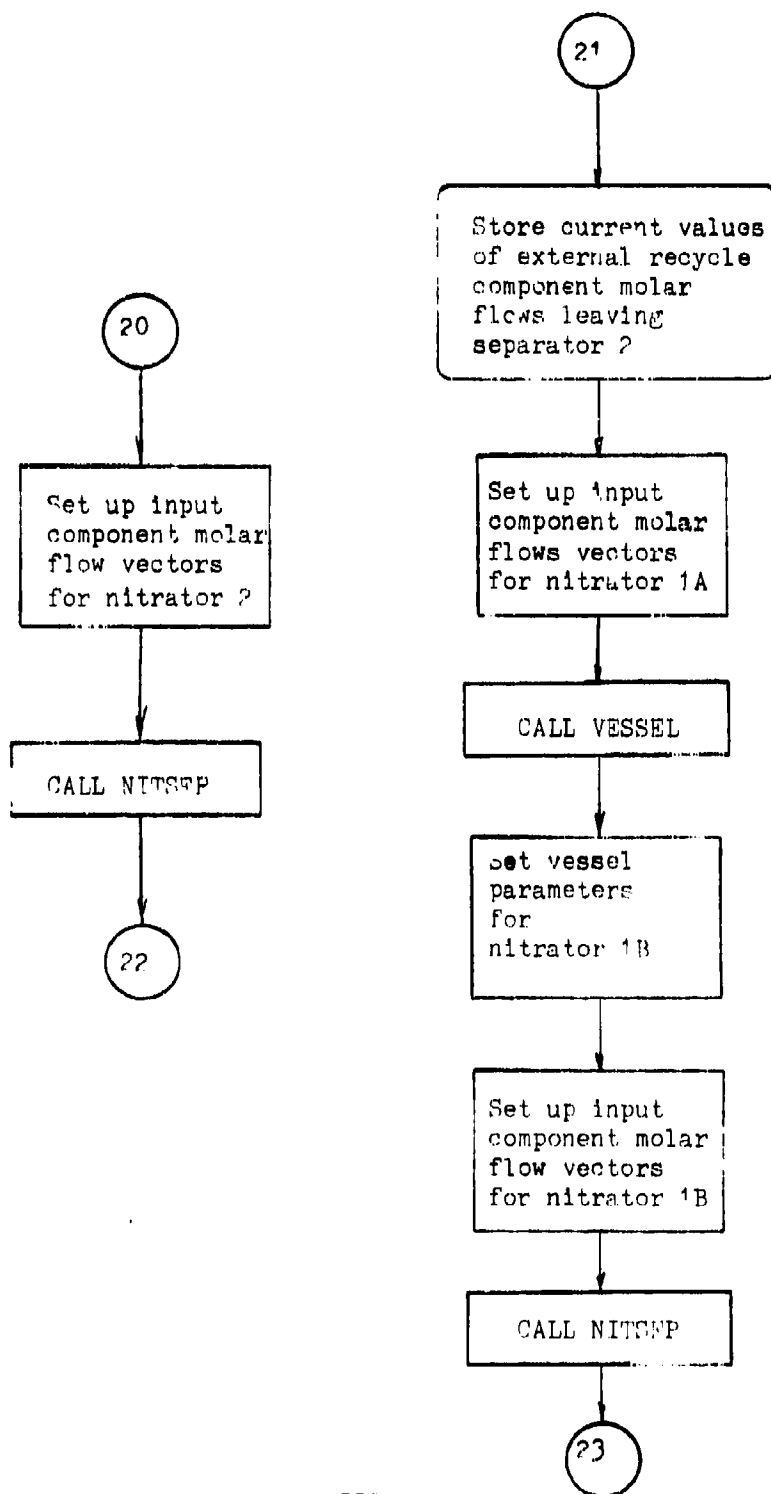


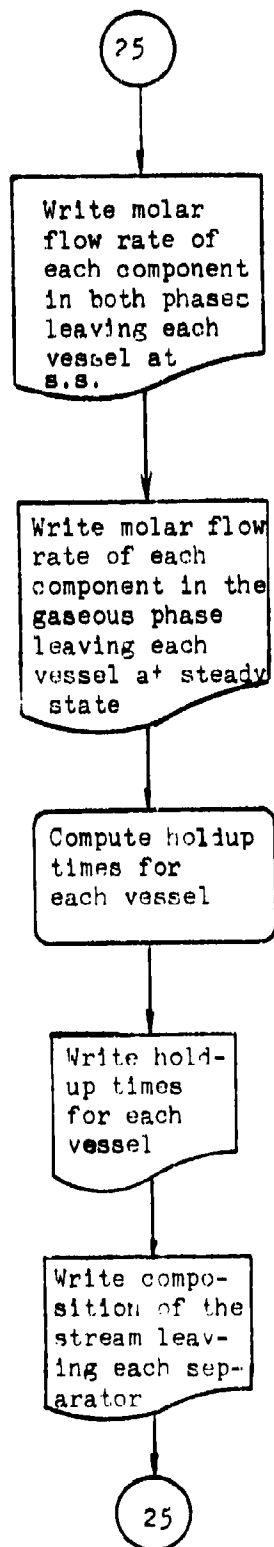


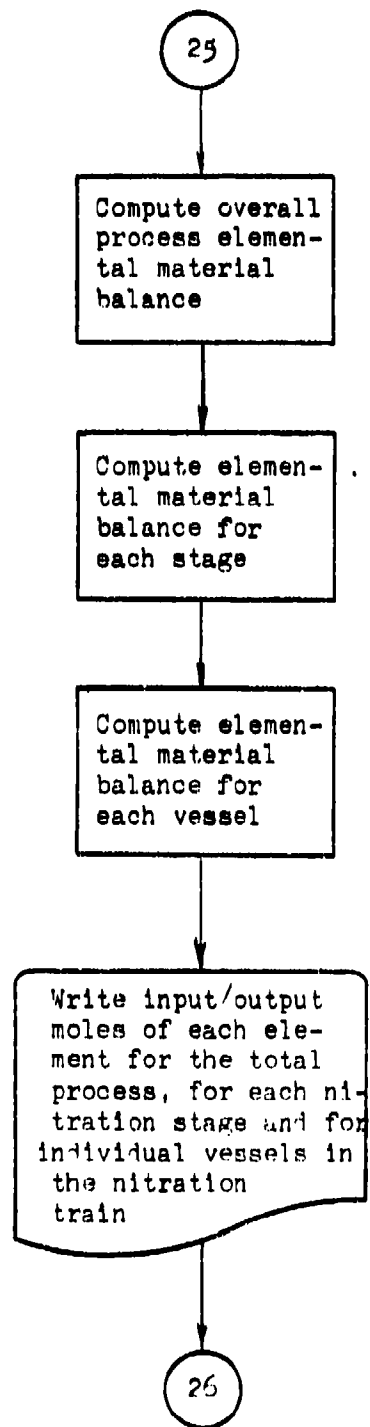












26

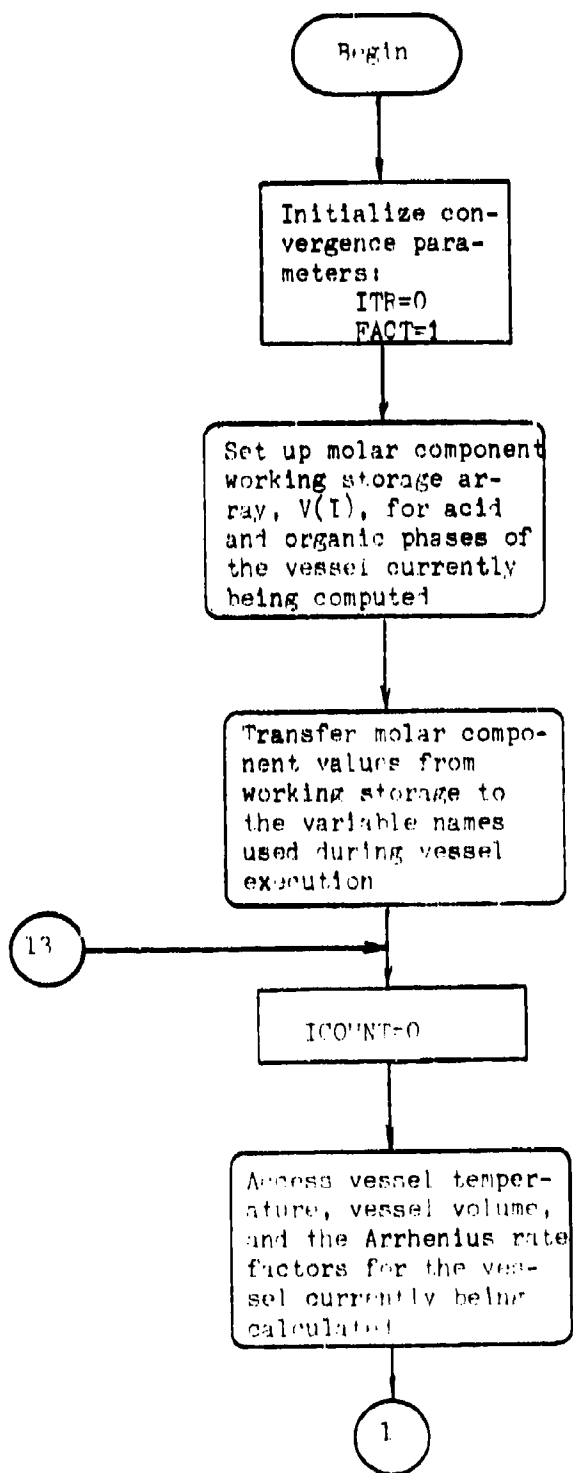
Compute process performance indicators including yield, crude TNT flow, product purity, raw materials cost, and spent acid flow and composition

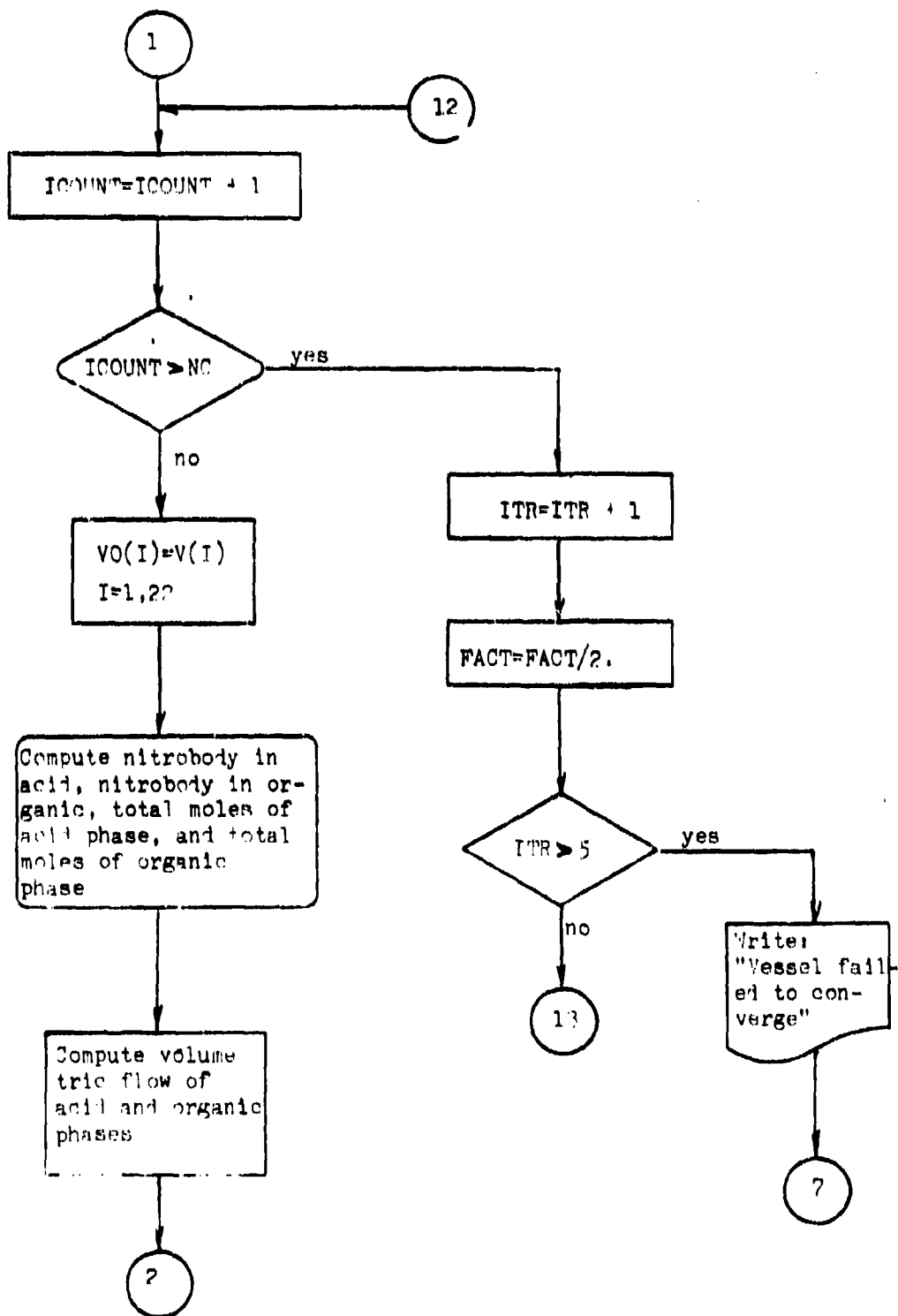
Compute stage performance indicators including extent of nitration, nitrating acid composition, nitrobody density and nitrator heat duties

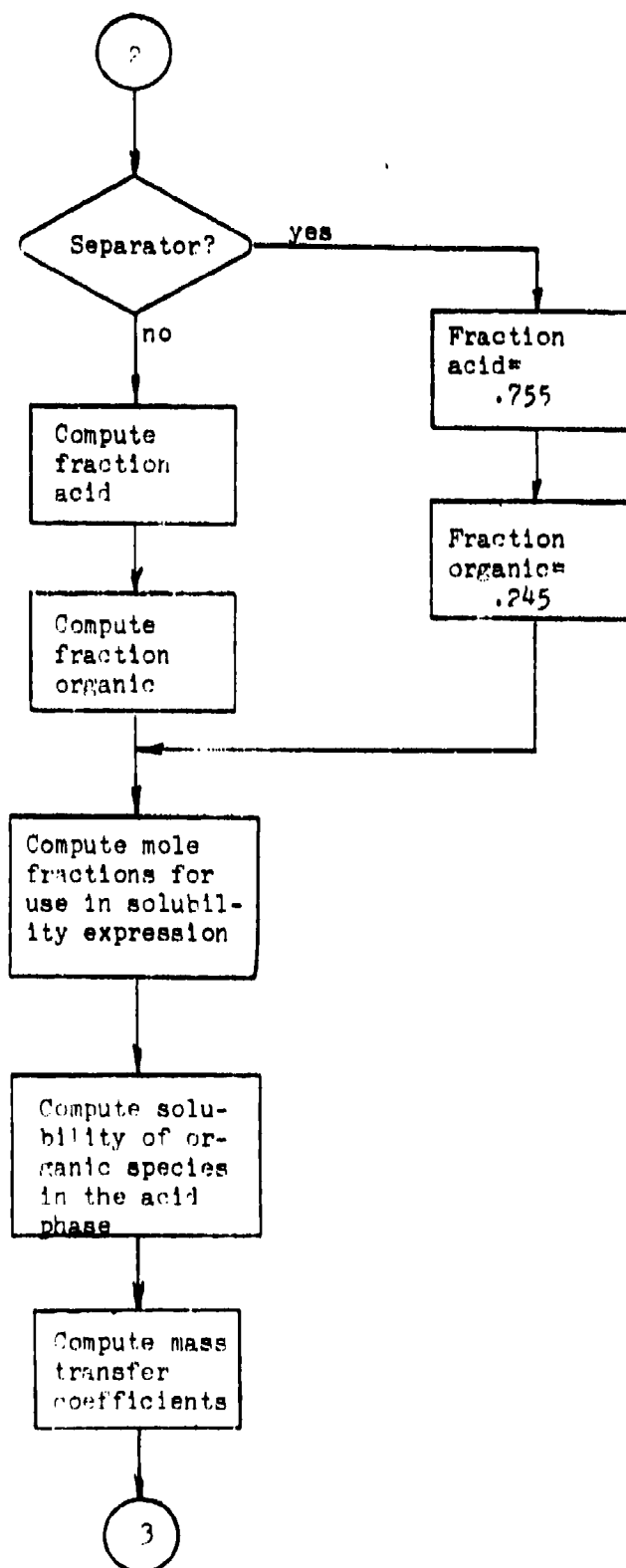
Write values of all performance indicators

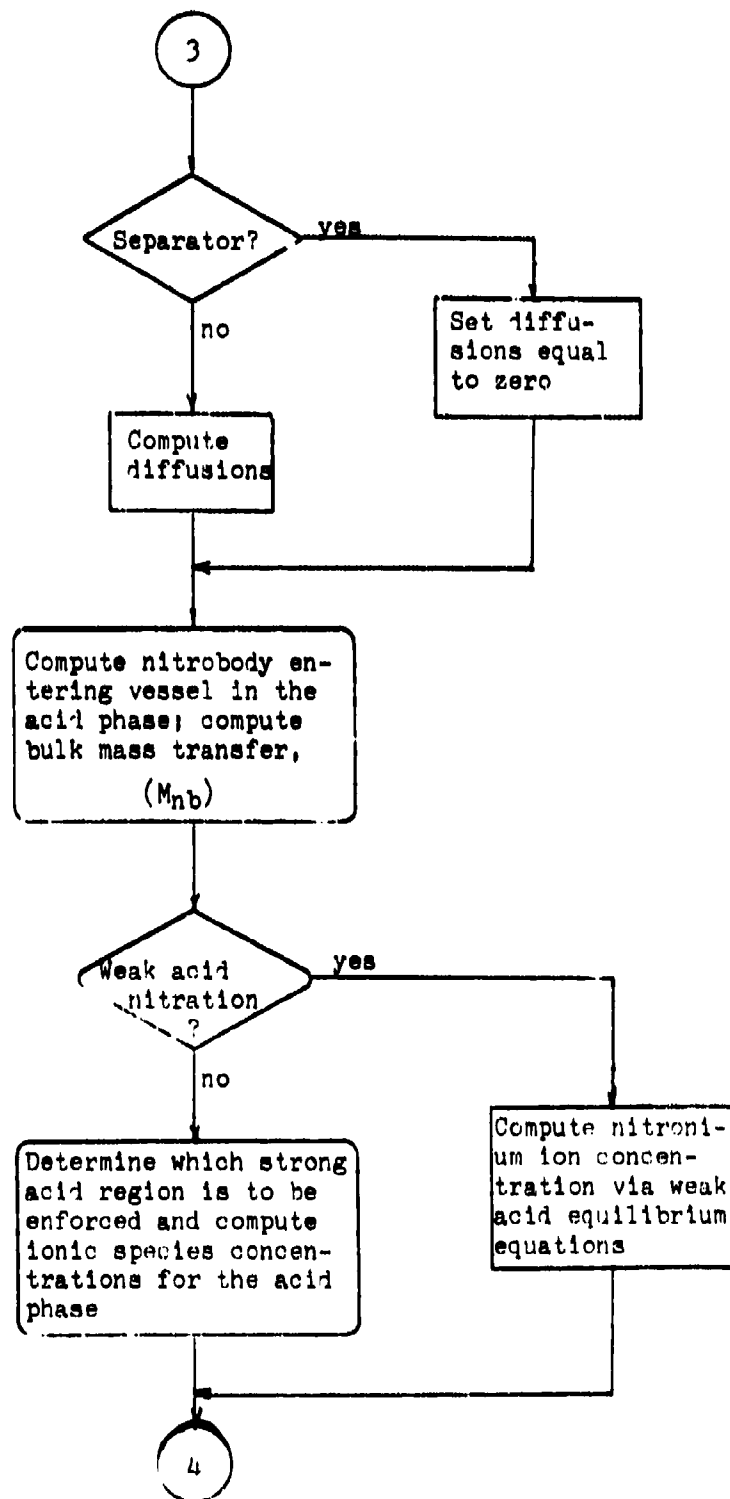
27

Subroutine VESSEL

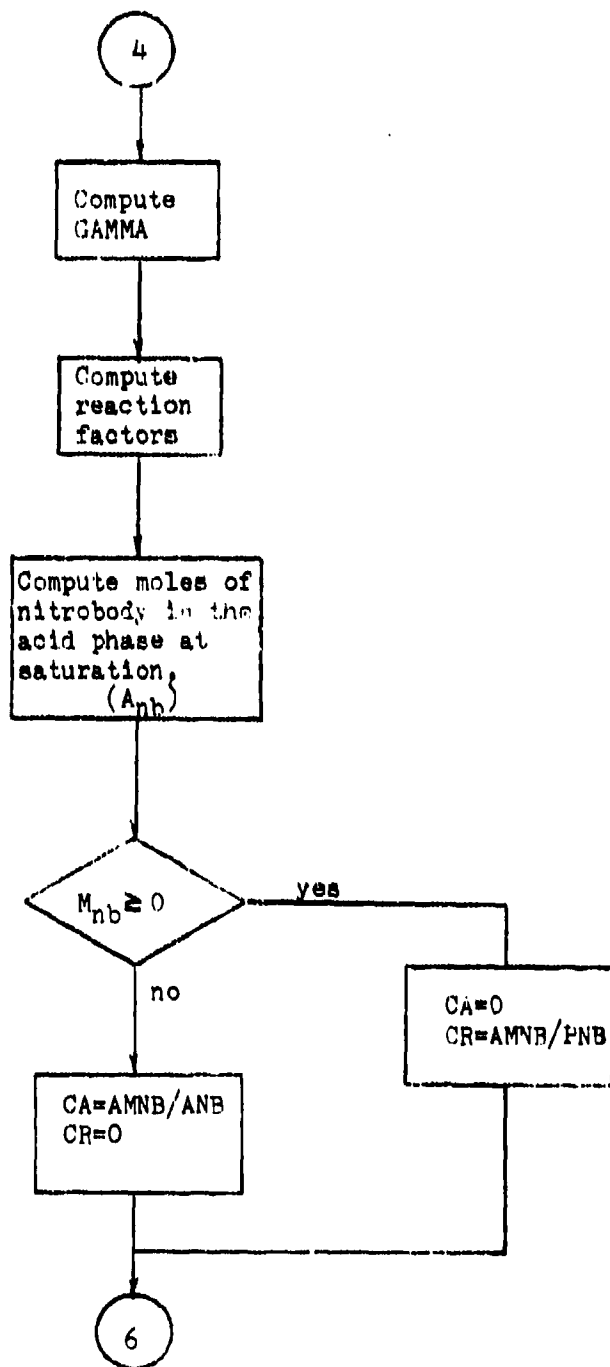


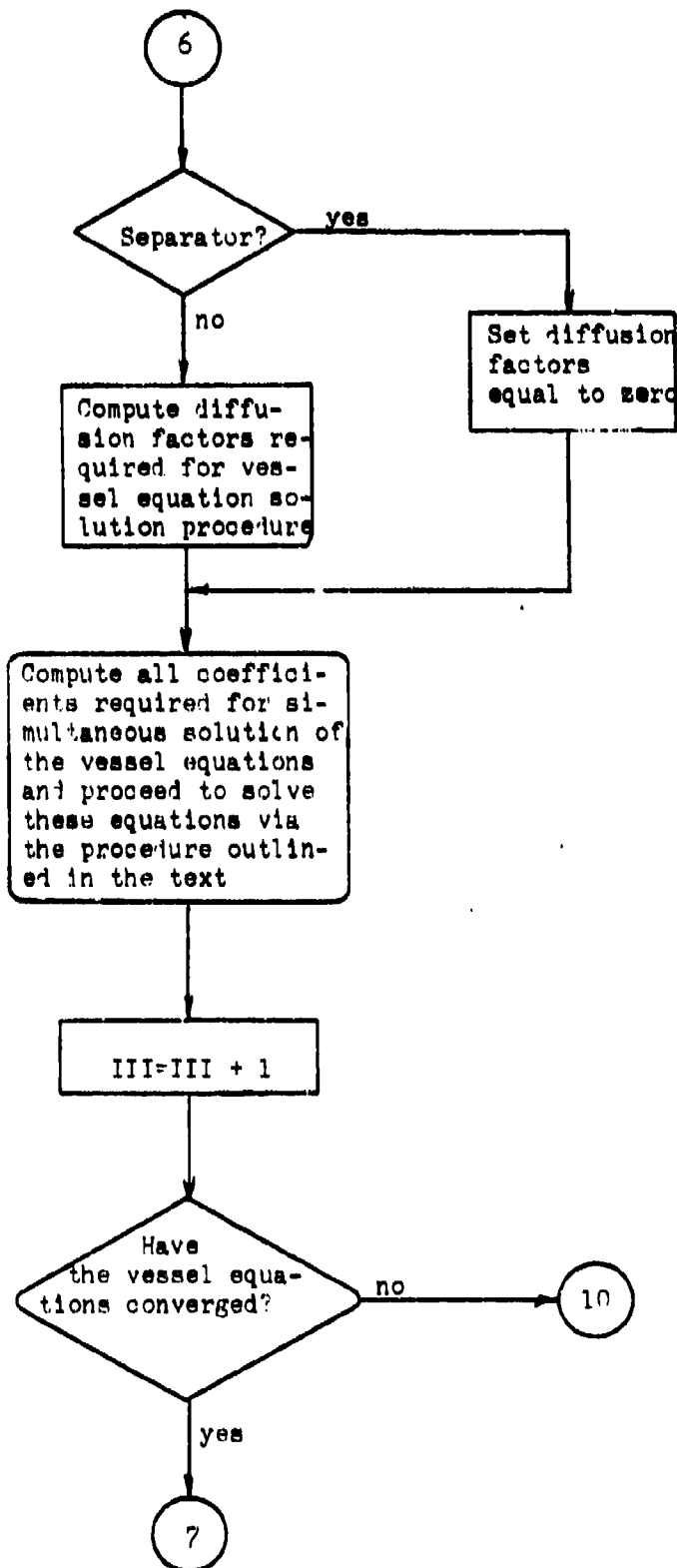


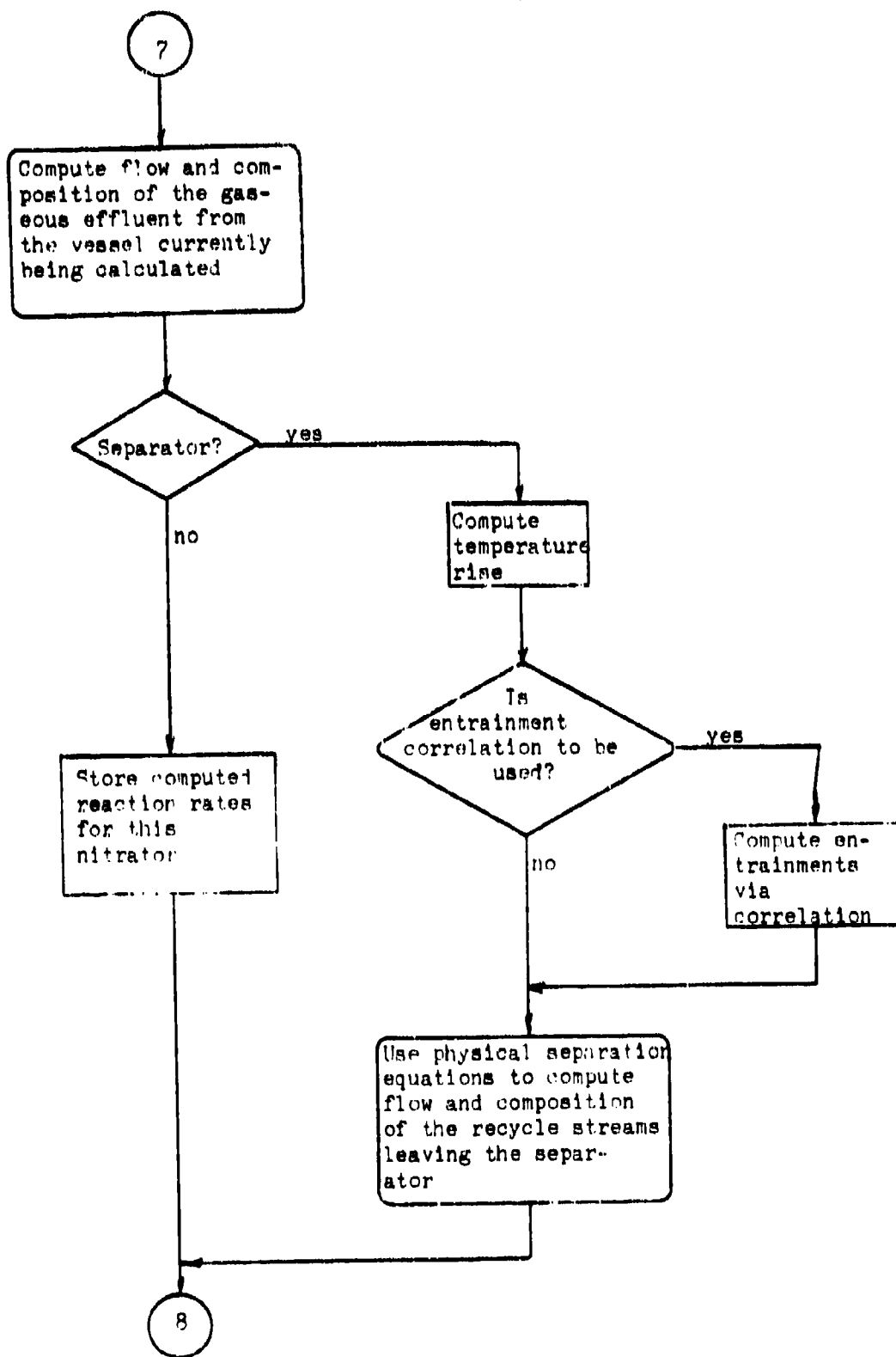


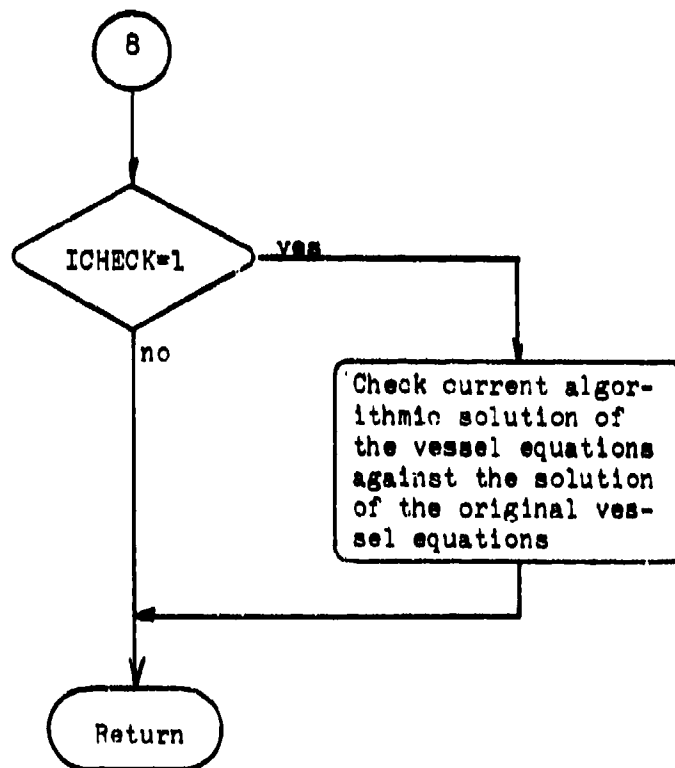


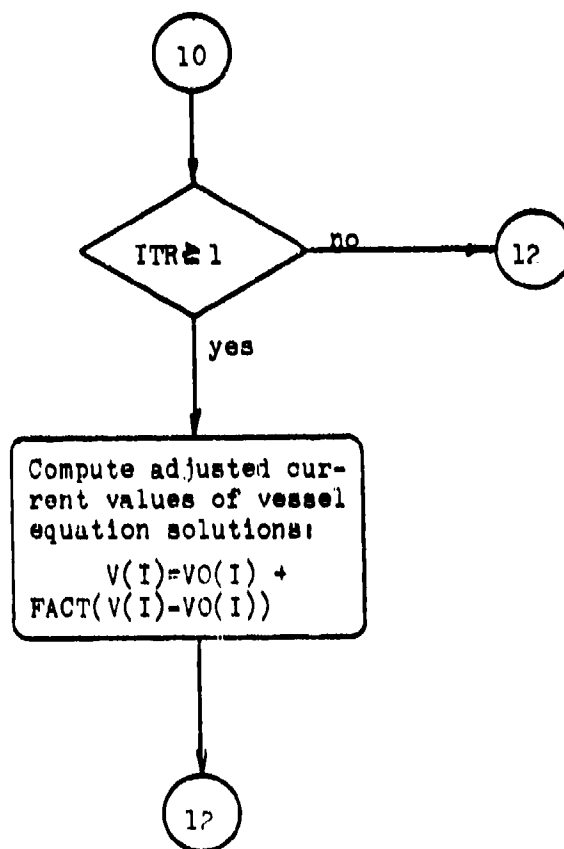
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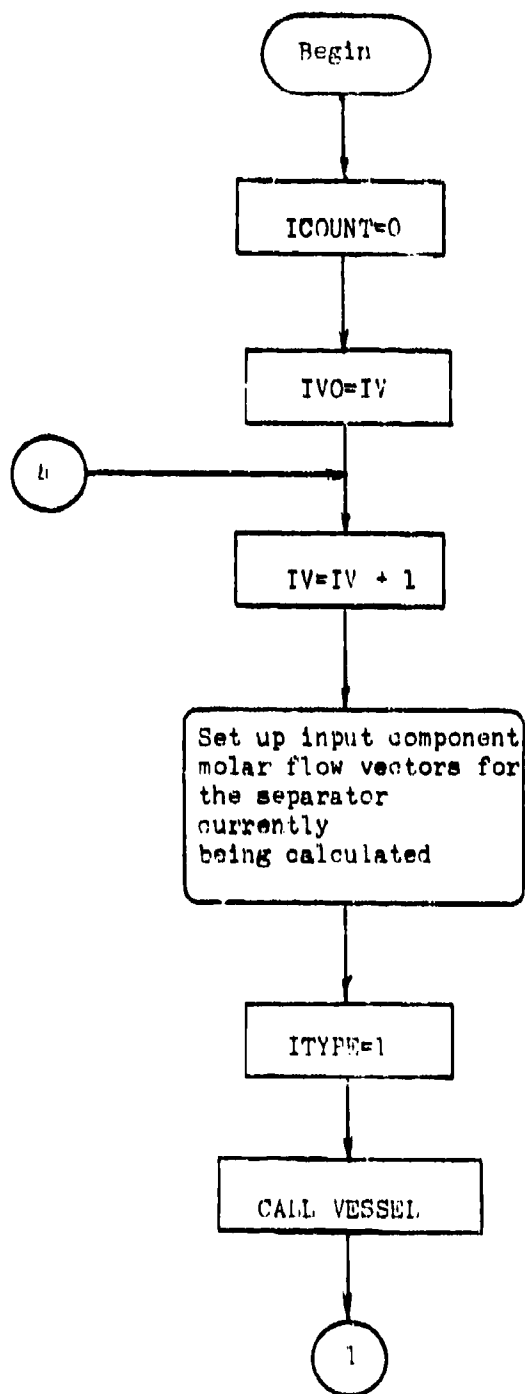


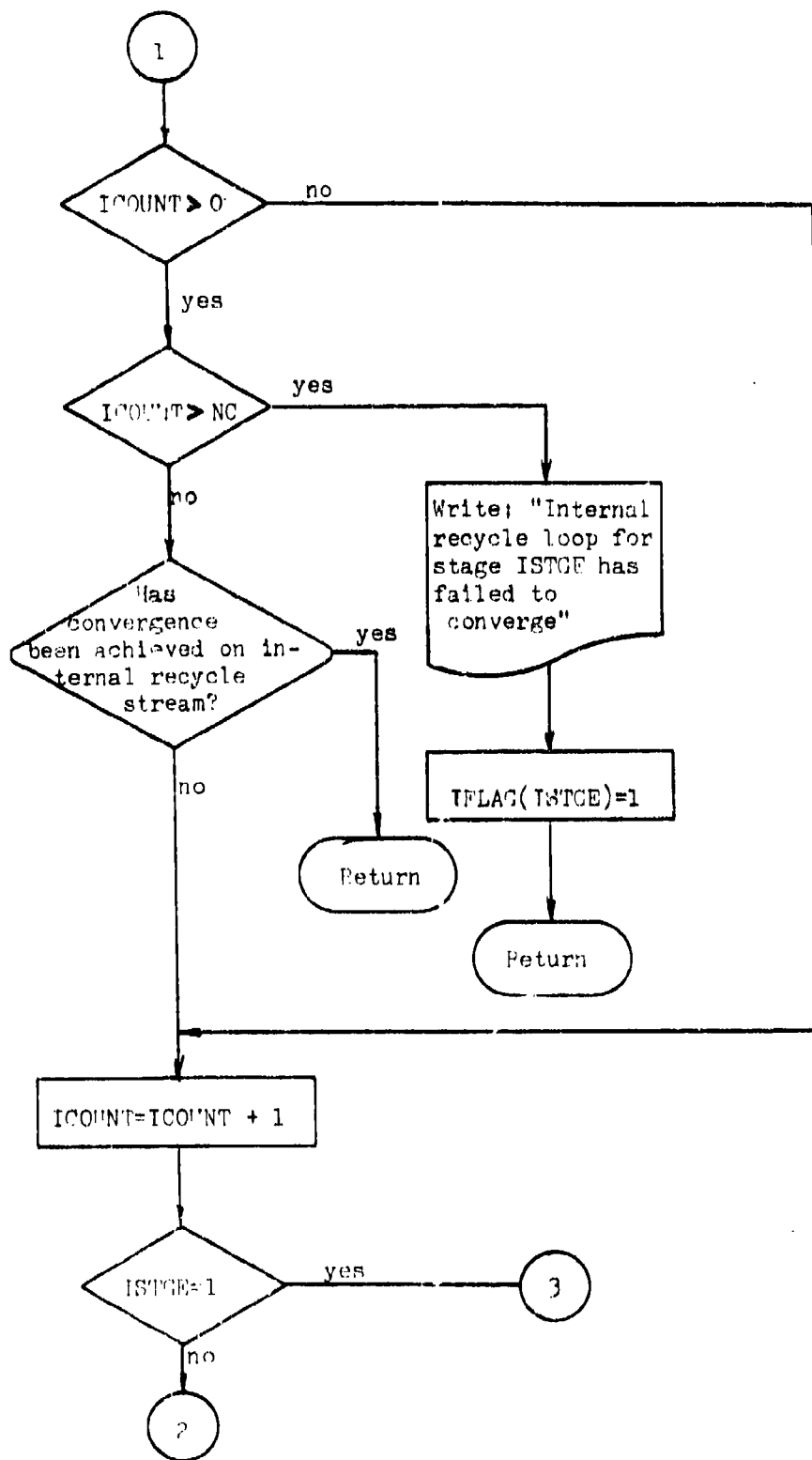


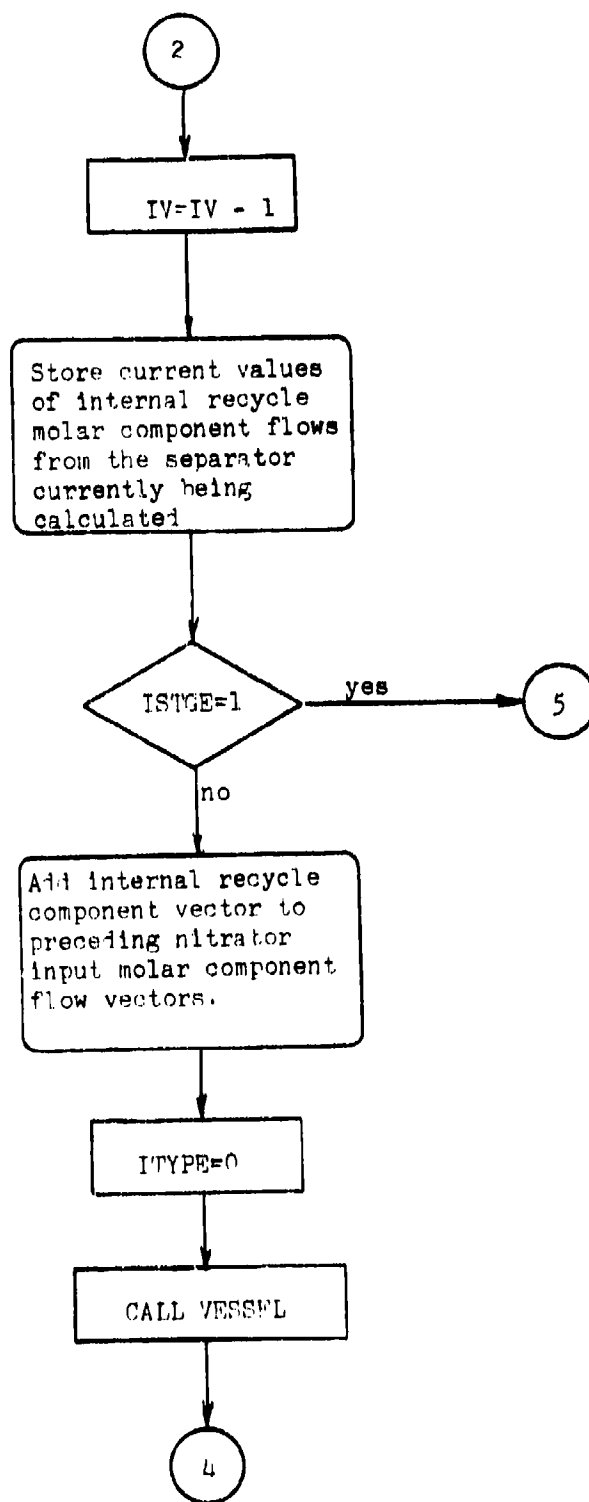


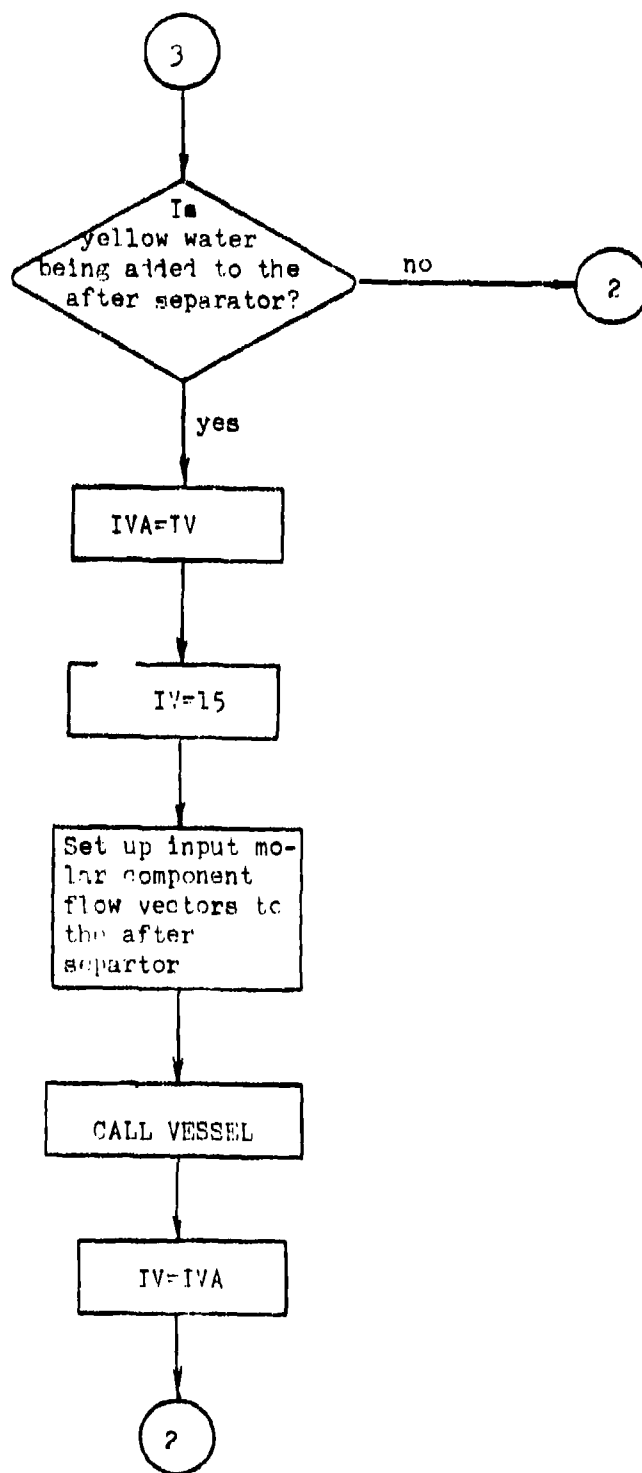


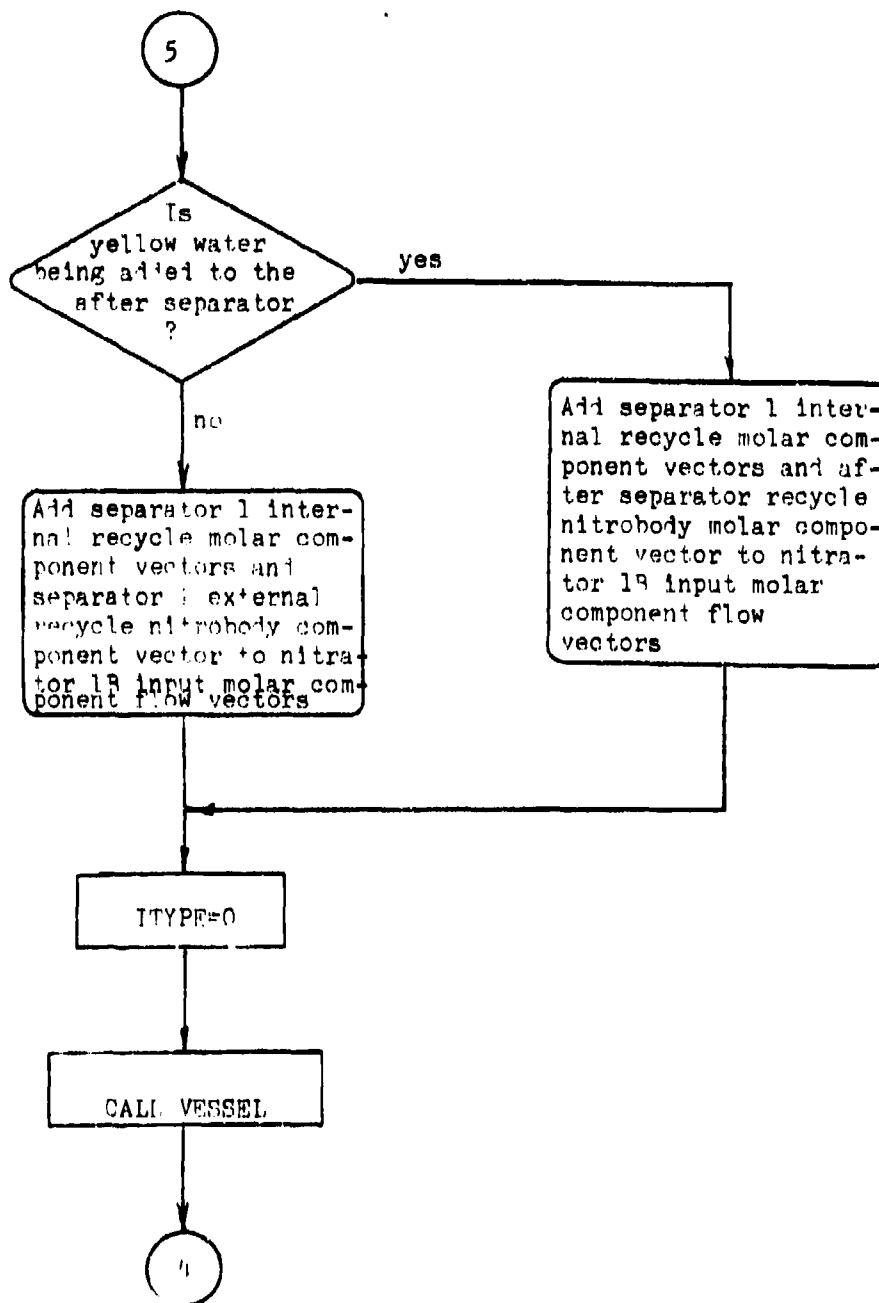
Subroutine NITSEP

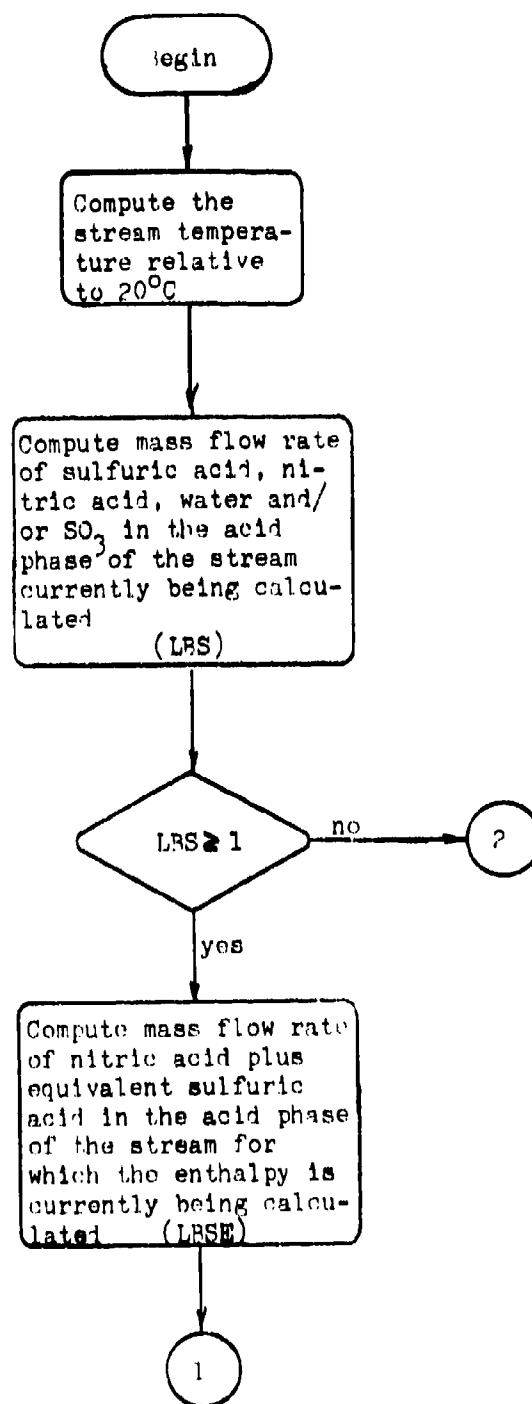


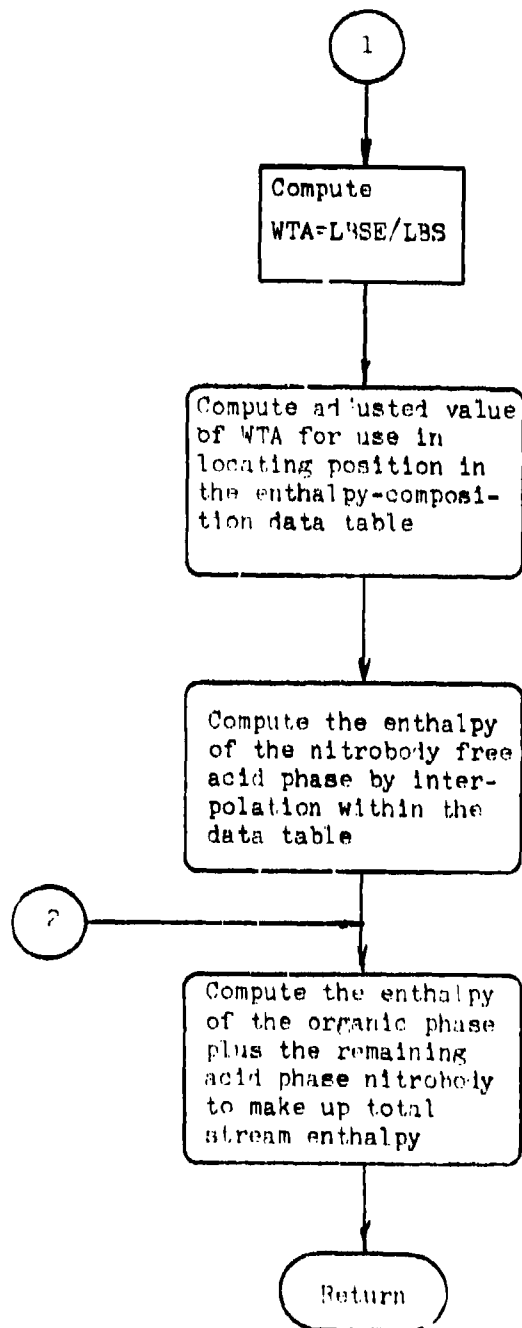












APPENDIX H

Steady State Simulation--Program Nomenclature

Main Program

AAS (I)	moles/hr of component i in the acid phase flowing from the after separator
AB	extent of nitration (either α or m) across the stage currently being calculated (moles/hr NO_2^+ added to the ring)
AF (I,J)	moles/hr of component i in the entrained acid phase of the organic stream flowing from separator j
AFLBS (I,J)	same as AF but in units of lbs/hr
AF1 (I)	moles/hr of component i in the entrained acid phase of the organic stream flowing from separator 1
AF2 (I)	same as AF1 but for separator 2
AF3 (I)	same as AF1 but for separator 3
AF4 (I)	same as AF1 but for separator 4
AF5 (I)	same as AF1 but for separator 5
AF6 (I)	same as AF1 but for separator 6
AI (I)	total acid phase moles/hr of component i flowing into a nitrator which is followed by another nitrator
AII (I)	total acid phase moles/hr (less acid phase of internal recycle) of component i flowing into a nitrator which is followed by a separator
AIR (I,J)	moles/hr of component i in the acid phase of the internal recycle stream flowing from separator j



AIR LBS (I,J)	same as AIR but in units of lbs/hr
AIR1 (I)	moles/hr of component i in the acid phase of the internal recycle stream flowing from separator 1
AIR2 (I)	same as AIR1 but for separator 2
AIR3 (I)	same as AIR1 but for separator 3
AIR4 (I)	same as AIR1 but for separator 4
AIR5 (I)	same as AIR1 but for separator 5
AIR6 (I)	same as AIR1 but for separator 6
AKA	general rate factor for all nitration reactions. Also, if Bennett's strong acid rate expression is used, the coefficient of the bisulfate ion concentration
AKB	coefficient of the sulfuric acid concentration in Bennett's rate expression
AKC	coefficient of the pyrosulfuric ion concentration in Bennett's rate expression
AKEQ	equilibrium constant for the sulfuric acid-water dissociation reaction
AKEQOV	equilibrium constant for the dissociation of a mixture of sulfuric and pyrosulfuric acids to ionic species. NOT USED
AKMA	acid phase mass transfer coefficient
AKMATL	mass transfer coefficient for toluene
AK10	rate constant for reaction 10
AK12	ratio of rate constants for reactions 1 & 2

AK3S	rate constant for reaction 3 in strong acid
AK3W	rate constant for reaction 3 in weak acid NOT USED
AK4S	rate constant for reaction 4 in strong acid
AK4W	rate constant for reaction 4 in weak acid NOT USED
AK5S	rate constant for reaction 5
AK6S	rate constant for reaction 6
AK7	rate constant for reaction 7
AK8	rate constant for reaction 8
AK9	NOT USED
AN(I)	percent actual nitric acid in the acid phase of the external recycle stream flowing from the <i>i</i> th separator
ANS(I)	mole fraction nitrosylsulfuric acid in the acid phase of the external recycle stream flowing from the <i>i</i> th separator
ANS1A	mole fraction nitrosylsulfuric acid in the acid phase flowing from nitrator 1A
ANS3A	mole fraction nitrosylsulfuric acid in the acid phase flowing from nitrator 3A
ARRAY(I,J)	moles/hr of component <i>i</i> in the raw material feedstocks flowing to nitrator <i>j</i>
AS(I)	percent sulfuric acid and SO ₃ (as equivalent sulfuric) in the acid phase of the external recycle stream flowing from the <i>i</i> th separator

0

AT	total moles/hr of acid phase flowing from the vessel for which the holdup is being computed
ATØM(I,J)	number of i-type atoms in component j
AV(I,J)	moles/hr of component i in the total acid phase flowing from vessel j
AVI(I,J)	first guess at converged value of moles/hr of component i in the acid phase flowing from vessel j
AXR(I,J)	moles/hr of component i in the acid phase of the external recycle stream flowing from separator j
AXRLBS(I,J)	same as AXR but in units of lbs/hr
AXR1(I)	moles/hr of component i in the acid phase of the external recycle stream flowing from separator 1
AXR2(I)	same as AXR1 but for separator 2
AXR2Ø(I)	previous value of AXR2(I) to which current value is compared during the external recycle convergence procedure
AXR3(I)	same as AXR1 but for separator 3
AXR3Ø(I)	same as AXR2Ø but for AXR3
AXR4(I)	same as AXR1 but for separator 4
AXR4Ø(I)	same as AXR2Ø but for AXR4
AXR5(I)	same as AXR1 but for separator 5
AXR5Ø(I)	same as AXR2Ø but for AXR5
AXR6(I)	same as AXR1 but for separator 6

AXR6Q (I)	same as AXR2Q but for AXR6
A1A (I)	moles/hr of component i in the total acid phase flowing from nitrator 1A
A1AI (I)	moles/hr of component i flowing into nitrator 1A from the raw material feedstocks
A1B (I)	same as A1A but for nitrator 1B
A1BI (I)	same as A1AI but for nitrator 1B
A1S (I)	moles/hr of component i in the total acid phase flowing from separator 1
A2 (I)	same as A1A but for nitrator 2
A2I (I)	same as A1AI but for nitrator 2
A2S (I)	same as A1S but for separator 2
A3A (I)	same as A1A but for nitrator 3A
A3AI (I)	same as A1AI but for nitrator 3A
A3B (I)	same as A1A but for nitrator 3B
A3BI (I)	same as A1AI but for nitrator 3B
A3S (I)	same as A1S but for separator 3
A4 (I)	same A1A but for nitrator 4
A4I (I)	same as A1AI but for nitrator 4
A4S (I)	same as A1S but for separator 4
A5 (I)	same as A1A but for nitrator 5
A5I (I)	same as A1AI bur for nitrator 5
A5S (I)	same as A1S but for separator 5

A6(I)	same as A1A but for nitrator 6
A6I(I)	same as A1AI but for nitrator 6
A6S(I)	same as A1S but for separator 6
BTU(I)	total heat load in nitrator 1, BTU/hr
BTUQ(I)	heat evolved in nitrator 1 which is due to chemical reaction only, BTU/hr
CDNT	weight % DNT in the nitrobody stream flowing from separator 6 on and acid free basis
COMP(I,J)	weight % component i in raw material feedstock type j
CP(I)	heat capacity of component i, BTU/lb-mole/°K
CRUDE	total mass flow rate (lbs/hr) of the organic stream from separator 6
CSL	cost of oleum, \$/lb
CSN	cost of strong nitric acid, \$/lb
CTF	cost of raw materials per unit of TNT produced, \$/lb α -TNT
CTL	cost of toluene, \$/lb
CWN	cost of weak nitric acid, \$/lb
DEL	convergence tolerance for components in acid recycle streams
DH(I)	heat of reaction for reaction i, BTU/lb-mole of reactant
DIF	storage variable for the difference between atoms of a given type in and atoms of that type out during material balance calculations

DLT	temperator of separator 1 referenced to 20°C
EAØ (I)	molar ratio of acid phase in the organic stream to total organic stream flowing from the i th separator
EAØP (I)	molar ratio of acid phase to organic phase in the organic stream flowing from the i th separator
EFR	enthalpy of mixing for fume recovery acid
EQA (I)	molar ratio of organic phase in the external recycle stream to the total external recycle stream flowing from the i th separator
EQAP (I)	molar ratio of organic phase to acid phase in the external recycle stream flowing from the i th separator
EØL	enthalpy of mixing for oleum
EWN	enthalpy of mixing for weak nitric acid
EYW'	enthalpy of mixing for yellow water
E10	activation energy for reaction 10
E21	ratio of activation energy for reaction 2 to that of reaction 1
E3S	activation energy for reaction 3
E3W	NOT USED
E4S	activation energy for reaction 4
E4W	NOT USED
E5S	activation energy for reaction 5
E6S	activation energy for reaction 6

E7	activation energy for reaction 7
E8	activation energy for reaction 8
E9	NOT USED
FA	volume fraction of acid phase in the vessel for which holdup is being calculated
FACD(I)	NOT USED
FACT2	relaxation factor used in convergence of the external recycle from separator 2
FACT3	same as FACT2 but for separator 3
FACT4	same as FACT2 but for separator 4
FACT5	same as FACT2 but for separator 5
FACT6	same as FACT2 but for separator 6
FD	extent of reaction for the decomposition of nitrosylsulfuric acid
FDN	moles/hr of ring associated NO ₂ groups flowing into a nitration stage with the organic stream from the previous stage
FIN (I,J)	lbs/hr of feedstock i to nitration vessel j
FMAX	maximum possible volumetric flow rate of material through any internal recycle pipe
FQ	volume fraction of organic phase in the vessel for which holdup is being calculated
FQV	NOT USED
GA (I,J)	number of i-type atoms in gaseous product j

CGS (I,J)	moles/hr of gaseous product j evolved in vessel i
G1 (I)	ratio of the Arrhenius coefficients in the kinetic rate expressions for reactions 1 and 2 in the i th nitrator
G10 (I)	Arrhenius coefficient for reaction 10 in nitrator i
G15 (I)	moles/hr of CO _{1,5} evolved from vessel i
G16 (I)	moles/hr of NO _x evolved from vessel i
G18 (I)	moles/hr of TNM evolved from vessel i
G19 (I)	moles/hr of CO ₂ evolved from vessel i
G3 (I)	NOT USED
G3S (I)	Arrhenius coefficient for reaction 3 in nitrator i
G4 (I)	NOT USED
G4S (I)	same as G3S but for reaction 4
G5 (I)	same as G3S but for reaction 5
G6 (I)	same as G3S but for reaction 6
G7 (I)	same as G3S but for reaction 7
G8 (I)	same as G3S but for reaction 8
G9 (I)	Zero
HDR (I,J)	array used to store alphanumeric headings for chemical elements in material balance printout
I	general index integer
LAFT	after separator switch. If equal to 1 then after separator is considered in the simulation as a dilution vessel to which 1000 lb/hr of yellow water is added

ICHECK	check calculation switch. If equal to 1 then check calculations are performed on the vessel equations in SUBROUTINE VESSEL
IE	entrainment correlation switch. If equal to 0 then entrainment correlation is used instead of assuming fixed values for entrainments
IFLG (I)	set equal to 1 whenever internal recycle loop for stage i does not converge
II	index used in calculation of extent of nitration in each stage
III	number of passes through SUBROUTINE VESSEL required to reach a converged solution
IJ	index used in calculation of extent of nitration in each stage
ILIST	printout switch. If equal to 1 printout of phase compositions, gas flows, vessel time constants, volumetric flows, acid phase solubility, vessel holdups and stream compositions is obtained
IMBAL	material balance switch. If equal to 1 chemical element balances are carried out on the entire nitration section, each individual nitration stage, and each individual vessel
IN	nitrator number
INIT (I)	vessel index. Has value of 1 if vessel is a nitrator and 0 if vessel is a separator
IPI	intermediate printout switch. If equal to 1 a printout of external recycle molar component flows after each iteration will be given

IPNCH	punch switch. If equal to zero no punched output. If equal to 1 final steady state (i.e. values of component molar flows for both phases in each vessel) is punched out for use as initial conditions in dynamic simulation or new first guess in steady state simulation
IPRNT	SUBROUTINE VESSEL printout switch. If equal to 1 gives a variety of debug printout which can be used to analyze problems associated with the vessel equations
ISTGE	stage number
ISTOP	equal to number of data sets plus 1. Program execution is terminated when NSET = ISTOP
ITYPE	equal to 0 for a nitrator and 1 for a separator
IV	vessel number
IV1	vessel number used during initial determination of recycle streams from first guess values of component molar phase flows
IX	index used in calculation of extent of nitration in each stage
IY	index used in calculation of extent of nitration in each stage
J	general index integer used for a variety of counting purposes
K	general index integer used for a variety of counting purposes
KEY	index which indicates whether extent of alpha or meta nitration is to be determined in a given stage
L	vessel index used in holdup calculation printout



M	vessel index used in holdup calculation printout
MHQLDA	total moles of acid phase holdup in the vessel currently being calculated
MHQLDQ	total moles of organic phase holdup in the vessel currently being calculated
MW(I)	molecular weight of component i
NATM	index of atomic species used in elemental material balance calculations
NC	maximum number of iterations allowed on any given recycle (internal or external) convergence loop
NC1	running sum of iterations on external recycle loop for separator 2
NC2	running sum of iterations on external recycle loop for separator 3
NC3	running sum of iterations on external recycle loop for separator 4
NC4	running sum of iterations on external recycle loop for separator 5
NC5	running sum of iterations on external recycle loop for separator 6
NDS	number of sets of operating conditions for which a steady state solution is desired in a given simulation run
NQ(I)	notch setting on the internal recycle gate valve for separator i
NET	number of the data set for which the steady state solution is currently being determined

NTOS (I)	molar ratio of nitric acid to the sum of sulfuric acid and SO_2 in the external recycle stream flowing from the i th separator
NTOS1A	molar ratio of nitric acid to the sum of sulfuric acid and SO_2 in the acid phase flowing from nitrator 1A
NTOS3A	same as NTOS1A but for nitrator 3A
QUTN	moles/hr of ring associated NO_2 groups flowing out of a given nitration stage
PACID (I,J)	pounds of component i held up in the acid phase of vessel j
PAS (I)	moles/hr of component i in the organic phase flowing from the after separator
PCTAS	weight % dissolved nitrobody in the acid phase flowing from the after separator under the condition of 1000 lb/hr of yellow water added to the after separator
PCTD	weight % DNT in the organic components dissolved in the acid phase flowing from separator 1
PCTNB	weight % total nitrobody contained in the acid stream flowing from separator 1 to the after separator
PCTNBD	weight % dissolved nitrobody contained in the acid stream flowing from separator 1 to the after separator
PF (I,J)	moles/hr of component i in the organic phase of the organic stream flowing from separator j
PFLBS (I,J)	same as PF but in units of lb/hr

PF1(I)	moles/hr of component 1 in the organic phase of the organic stream flowing from separator 1
PF2(I)	same as PF1 but for separator 2
PF3(I)	same as PF1 but for separator 3
PF4(I)	same as PF1 but for separator 4
PF5(I)	same as PF1 but for separator 5
PF6(I)	same as PF1 but for separator 6
PI(I)	total organic phase moles/hr of component 1 flowing into a nitrator which is followed by another nitrator
PII(I)	total organic phase moles/hr of component 1 (less organic phase of internal recycle) flowing into a nitrator which is followed by another separator
PIR(I,J)	moles/hr of component 1 in the organic phase of the internal recycle stream flowing from separator j
PIRLBS(I,J)	same as FIR but in units of lb/hr
PIR1(I)	moles/hr of component 1 in the organic phase of the internal recycle stream flowing from separator 1
PIR2(I)	same as PIR1 but for separator 2
PIR3(I)	same as PIR1 but for separator 3
PIR4(I)	same as PIR1 but for separator 4
PIR5(I)	same as PIR1 but for separator 5
PIR6(I)	same as PIR1 but for separator 6

PNS	weight % nitrosylsulfuric acid in the acid phase of the external recycle stream flowing from a given separator
POUNDS (I,J)	pounds of component i held up in the organic phase of vessel j
PT	total moles/hr of organic phase flowing from the vessel for which the holdup is being computed
PV (I,J)	moles/hr of component i in the total organic phase flowing from vessel j
PVI (I,J)	first guess at converged value of moles/hr of component i in the organic phase flowing from vessel j
PXR (I,J)	moles/hr of component i in the organic phase of the external recycle stream flowing from separator j
PXRLBS (I,J)	same as PXR but in units of lb/hr
PXR1 (I)	moles/hr of component i in the organic phase of the external recycle stream flowing from separator 1
PXR2 (I)	same as PXR1 but for separator 2
PXR2Q (I)	previous value of PXR2 (I) to which current value is compared during the external recycle convergence procedure
PXR3 (I)	same as PXR1 but for separator 3
PXR3Q (I)	same as PXR2Q but for separator 3
PXR4 (I)	same as PXR1 but for separator 4
PXR4Q (I)	same as PXR2Q but for separator 4
PXR5 (I)	same as PXR1 but for separator 5
PXR5Q (I)	same as PXR2Q but for separator 5

PXR6 (I)	same as PXR1 but for separator 6
PXR80 (I)	same as PXR20 but for separator 6
P1A (I)	moles/hr of component i in the total organic phase flowing from nitrator 1A
P1AI	moles/hr toluene to nitrator 1A
P1B (I)	same as P1A but for nitrator 1B
P1BI	moles/hr toluene to nitrator 1B
P1S (I)	moles/hr of component i in the total organic phase flowing from separator 2
P2 (I)	moles/hr of component i in the total organic phase flowing from nitrator 2
P2S (I)	same as P1S but for separator 2
P3A (I)	same as P2 but for nitrator 3A
P3B (I)	same as P2 but for nitrator 3B
P3S (I)	same as P1S but for separator 3
P4 (I)	same as P2 but for nitrator 4
P4S (I)	same as P1S but for separator 4
P5 (I)	same as P2 but for nitrator 5
P5S (I)	same as P1S but for separator 5
P6 (I)	same as P2 but for nitrator 6
P6S (I)	same as P1S but for nitrator 6
Q	accumulation term used in calculation of nitrator heat loads

QA	ft ³ /hr of total acid phase flowing from the vessel for which holdup is being computed
QP	same as QA but for organic phase
QQ(I)	fraction nitric acid converted to nitronium ion in vessel i
QT	ft ³ /hr of total material flowing from the vessel for which holdup is being computed
R(I)	rate of reaction for reaction i in the vessel currently being simulated by SUBROUTINE VESSEL
RATES(I,J)	rate of reaction for reaction j in nitrator i
REC�	moles/hr of ring associated NO ₂ groups flowing into a nitration stage with the external recycle from the next higher stage
RHQ(I)	molar density of component i
RHQA	molar density of the acid phase in the vessel for which holdup is being calculated
RHQNBS(I)	mass density of the nitrobody dissolved in the acid phase of the external recycle stream flowing from the i th separator
RHQP	molar density of the organic phase in the vessel for which holdup is being calculated
RHQ1	equivalent to RHQ(1)
RHQ10	equivalent to RHQ(10)
RHQ11	equivalent to RHQ(11)
RHQ12	equivalent to RHQ(12)
RHQ13	equivalent to RHQ(13)

RHQ14	equivalent to RHQ (14)
RHQ2	equivalent to RHQ (2)
RHQ3	equivalent to RHQ (3)
RHQ4	equivalent to RHQ (4)
RHQ5	equivalent to RHQ (5)
RHQ6	equivalent to RHQ (6)
RHQ7	equivalent to RHQ (7)
RHQ8	equivalent to RHQ (8)
RHQ9	equivalent to RHQ (9)
RP	coefficient of the molecular oxygen term in reaction 9
RPP	precomputed constant based on RP which is used in material balance calculations
RR	ideal gas law constant
SA	adjustable constant. NOT USED
SB	equivalent to KMAP
SC	equivalent to AKEQ4 in SUBROUTINE VESSEL
SD	adjustable constant. NOT USED
SE	equivalent to AK9. NOT USED
SG	equivalent to E9. NOT USED
SH	equivalent to AKEQ1 in SUBROUTINE VESSEL
SI	adjustable constant. NOT USED

SJ	equivalent to AKEQ3 in SUBROUTINE VESSEL
SNA (I)	net moles/hr of ring associated alpha NO ₂ groups flowing through the i th nitration stage. Extent of alpha-nitration in nitration stage i
SNM (I)	same as SNA but for meta-nitration
SOL (I)	saturation solubility of total organic components in the acid phase of vessel i
SPA	mass flow rate of the acid phase of the external recycle stream (spent acid) from separator 1
SPACID	mass flow rate of the total external recycle stream from separator 1
SPP	mass flow rate of the organic phase of the external recycle stream from separator 1
STN	total flow rate (lb/hr) of strong nitric acid into the process from all raw material feed streams
SULP	total flow rate (lb/hr) of oleum into the process from all raw material feed streams
SUM	total molar flow rate of gasses evolved in the nitration stage for which material balance calculations are being executed. Also the moles/hr of organics flowing from separator 6 with the organic stream
SUMA	mass flow rate acid components of the acid phase from the after separator when the after separator option is used
SUMI	accumulation term for input streams used during material balance calculations (moles/hr)
SUMØ	mass flow rate of organic components in the acid phase from the after separator when the after separator option is used

S15	total moles/hr of $\text{CO}_{1.8}$ evolved in nitration section
S16	total moles/hr of NO_x evolved in the nitration section
S18	total moles/hr of TNM evolved in the nitration section
S19	total moles/hr of CO_2 evolved in the nitration section
TANB	total moles/hr of dissolved organics in the acid phase of the external recycle flowing from separator 1
TAS (I)	total acidity of the acid phase of the external recycle stream flowing from separator 1
TATMI	total moles/hr of a given atomic specie entering that section of the process over which an elemental material balance is being computed
TATMØ	total moles/hr of a given atomic specie exiting that section of the process over which an elemental material balance is being computed
TAU	holdup time in a given vessel
TCØX	equivalent to S15
TCO2	equivalent to S19
TDNT	total mass flow rate of DNT in the organic stream from separator 6
TDNTA	total pounds of DNT held up in the acid phase of all process vessels
TDNTP	total pounds of DNT held up in the organic phase of all process vessels

TEMP (I)	temperature of the i^{th} nitrator
TITLE (I)	alphanumeric identifying information for a given data set
TLBS	total lb/hr of acid components in the acid phase of the external recycle stream flowing from the separator for which acid composition calculations are being executed
TMQLES	same as TLBS but in units of moles/hr
TN (I)	weight % total nitric acid in the acid phase of the external recycle stream flowing from the i^{th} separator on an organic free basis
TNOX	equivalent to S16
TNTI	moles/hr of TNT entering the nitration section with feed material
TOL	lb/hr toluene fed to the nitration section
TPNB	total moles/hr of organic components in the organic phase of the external recycle stream flowing from separator 1
TPOUND	accumulation term for total pounds of organic material held up in either the acid or organic phase of the vessel for which holdup calculations are being executed
TR	reference temperature
TS (I)	weight % total sulfuric acid plus SO_3 (as equivalent sulfuric) in the acid phase of the external recycle stream flowing from the i^{th} separator on an organic free basis
TSEP (I)	temperature of the i^{th} separator
TSEP1	equivalent to TSEP (1)

TSEP2	equivalent to TSEP (2)
TSEP3	equivalent to TSEP (3)
TSEP4	equivalent to TSEP (4)
TSEP5	equivalent to TSEP (5)
TSEP6	equivalent to TSEP (6)
TTDNT	total pounds of DNT held up in all process vessels
TTLBS (I)	total pounds of organic phase held up in the ith vessel
TTLBSA (I)	total pounds of organic components held up in the acid phase of the ith vessel
TTNM	equivalent to S18
TTNTA	total pounds of TNT held up in the acid phase of all process vessels
TTNTP	total pounds of TNT held up in the organic phase of all process vessels
TTTLBA	total pounds of organic components held up in the acid phase of all process vessels between and including nitrator 2 and separator 6
TTTLBS	total pounds of organic phase held up in all process vessels between and including nitrator 2 and separator 6
TTTNT	total pounds of TNT held up in all process vessels
TTTTLB	total pounds of organic components (in both acid and organic phases) held up in all process vessels between and including nitrator 2 and separator 6
TVQL	volumetric flow of the organic compounds in the acid phase of the external recycle stream flowing from a separator for which nitrobody density is being computed

T1A	temperature of nitrator 1A
T1B	temperature of nitrator 1B
T2	temperature of nitrator 2
T3A	temperature of nitrator 3A
T3B	temperature of nitrator 3B
T4	temperature of nitrator 4
T5	temperature of nitrator 5
T6	temperature of nitrator 6
V (I)	storage vector for current values of the i component flow terms generated in SUBROUTINE VESSEL
VHOLDA	volume of acid phase held up in a given vessel
VHOLDQ	volume of organic phase held up in a given vessel
VKM (I)	working volume of the i th nitrator
VKMS	working volume of any separator
VOL (I)	working volume of the i th vessel
WKN	total flow rate (lb/hr) of weak nitric acid into the process from all raw material feed stream
XP (I,J)	mole fraction of component i in the organic phase within vessel j
XPA (I,J)	mole fraction of component i in the acid phase within vessel j
YELLOW (I)	moles/hr of component i in the yellow water fed to the after separator whenever the after separator option is chosen.

YIELD

moles α -TNT in the organic stream flowing from separator 6 per mole of toluene fed to the process (expressed as %)

ZA

temperature coefficient in the exponent of the Arrhenius rate law

Subroutine NITSEP

The definitions of the following variables are identical to those in the main program: AF(I,J), AF1(I), AI(I), AII(I), AIR(I,J), AIR1(I), AV(I,J), AXR(I), AXR1(I), DEL, EAQ(I), EAQP(I), EQA(I), EQAP(I), FACD(I), G15(I), G16(I), G18(I), G19(I), I, IAFI, ICHECK, IE, IFLG(I), IN, IPRNT, ISTGE, ITYPE, IV, NQ(I), PF(I,J), PF1(I), PI(I), PII(I), PIR(I,J), PIR1(I), PV(I,J), PXR(I), PXR1(I), RATES(I,J), SOL(I), TSEP(I), YELLOW(I),

Remaining variables are defined as follows:

AIRQ(I)

previous value of AIR(I,J) to which current value is compared during the internal recycle convergence procedure for stage j

ICOUNT

counter for iterations of internal recycle convergence loop

IVA

vessel index for separator 1 used whenever after separator is included in the simulation

IVQ

vessel index for the nitrator which precedes the separator for which internal recycle convergence is being executed

PIRQ(I)

previous value of PIR(I,J) to which current value is compared during the internal recycle convergence procedure for stage j

Subroutine VESSEL

The definitions of the following variables are identical to those in the main program: AF(I,J), AI(I), AIR(I,J), AKA, AKEQ, AKEQOV, AKMA, AKMAP, AKMATL, AK10, AK12, AK3S, AK3W, AK4S, AK4W, AK4S, AK6S, AK7, AK8, AV(I,J), AXR(I,J), CP(I), DEL, DH(I), EAQ(I), EAQP(I), EQA(I), EQAP(I), E10, E12, E3S, E3W, E4S, E4W, E5S, E6S, E7, E8, FACD(I,J), FP, FMAX, G15(I), G16(I), G18(I), G19(I), I, IAF, ICHECK, IE, III, IN, IPRNT, ISTGE, ITYPE, IV, J, MN(I), NQ(I), PF(I,J), PI(I), PIR(I,J), PV(I,J), PXR(I,J), QQ(I), R(I), RATES(I,J), RHQ1, RHQ10, RHQ12, RHQ13, RHQ14, RHQ2, RHQ3, RHQ4, RHQ5, RHQ6, RHQ7, RHQ8, RHQ9, RP, RR, SA, SB, SC, SD, SE, SG, SH, SI, SJ, SOL(I), TEMP(I), TR, TSEP(I), V(I), VKM(I), VKMS, YELLOW(I)

The definitions of the following variables are identical to other variables defined in the main program:

Variable in VESSEL

Variable in main program

AI1 thru AI17
F1(I) thru F10(I)
ISEP
PI1 thru PI17
R1 thru R10

AI(1) thru AI(17)
G1(I) thru G10(I)
ISTGE
PI(1) thru PI(17)
R(1) thru R(10)

Remaining variables are defined as follows:

A(I)	moles/hr of component i in the acid phase flowing from the vessel currently being simulated
AINB	moles/hr of organic components in the combined acid phase flowing to the vessel currently being simulated
AKEQ1	equilibrium constant for the dissociation of nitric acid in aqueous sulfuric acid
AKEQ2	equilibrium constant for the dissociation of sulfuric acid in an aqueous system
AKEQ3	equilibrium constant for dissociation of nitric acid in anhydrous sulfuric acid

AKEQ4	equilibrium constant for the recombination of nitronium and bisulfate ions in anydrous acid mixtures
AK1	computed value of AKEQ1 obtained from interval halving procedure
AK3	computed value of AKEQ3 obtained from interval halving procedure
AK4	computed value of AKEQ4 obtained from interval halving procedure
AL	moles/hr water in the acid phase flowing from the vessel currently being simulated; negative values represent moles/hr SO_3
AM (I)	moles/hr of component i transferred from the organic phase into the acid phase by bulk mass transfer in the vessel currently being simulated. Used in check calculations only
AMNB	total moles/hr of organic components transferred from the organic to acid phase by bulk mass transfer in the vessel currently being simulated
AM1	moles/hr α -MNT transferred from the organic phase into the acid phase by bulk mass transfer in the vessel currently being simulated
ANB	moles/hr organic components in the acid phase flowing from the vessel currently being simulated
ASØ4	combined moles/hr of H_2SO_4 and SO_3 in the acid phase flowing from the vessel currently being simulated
AT	total moles/hr of acid phase flowing from the vessel currently being simulated
ATI	reciprocal of AT

AXL	same as AL but used only in check calculations
AX1	1. + C1A-CA
AX1 thru AX9	same as A1 thru A9 but used only in check calculations
AX12	same as A12 but used only in check calculations
A1	moles/hr α MNT in the acid phase flowing from the vessel currently being simulated
A2	same as A1 but for m MNT
A3	same as A1 but for α DNT
A4	same as A1 but for m MNT
A5	same as A1 but for α TNT
A6	same as A1 but for m TNT
A7	same as A1 but for TNBX
A8	same as A1 but for TNB
A9	moles/hr nitric acid in the acid phase flowing from the vessel currently being simulated
A11	same as A9 but for H_2SO_4
A12	same as A9 but for nitrosylsulfuric acid
A13	same as A9 but for water
A14	same as A9 but for SO_3
A17	moles/hr nitronium ion in the acid phase flowing from the vessel currently being simulated
B	free sulfuric acid concentration in oleum in the vessel currently being simulated

BC	$B + (3 \times C)$
B1	term representing moles/hr of an organic component flowing into a vessel with the combined acid phase plus the amount of that component formed by reaction
B2	moles/hr of an organic component flowing into a vessel with the combined organic phase
C	concentration of pyrosulfuric acid in the vessel currently being simulated
CA	ratio of AMNB to ANB (constant used in determining bulk mass transfer during simultaneous solution of vessel equations)
CB	$(.5 \times B) + (1.5 \times C)$
CF	$C - F$
CHNØ3	equilibrium concentration of nitric acid in the acid phase of the vessel currently being simulated (moles/cf ³)
CHSØ4	same as CHNØ3 but for bisulfate ion
CHS2Ø7	same as CHNØ3 but for pyrosulfate ion
CH2Ø	same as CHNØ3 but for water
CH2SO4	same as CHNØ3 but for sulfuric acid
CH3Ø	same as CHNØ3 but for hydronium ion
CNØ2	same as CHNØ3 but for nitronium ion
CR	ratio of AMNB to PNB. Constant used in determination of bulk mass transfer during simultaneous solution of vessel equations
CVØL	computed volumetric flow of an internal recycle stream based on entrainment correlation

CXX	correlation used to determine fraction organic entrained in the internal recycle stream
CX2	ratio of fraction internal recycle to fraction external recycle used in entrainment correlation
C1	equal to overall mass transfer coefficient (ETA) during simultaneous solution of vessel equations
C1A	coefficient equal to $C1/ANB$ used during simultaneous solution of vessel equations
C1Ø	coefficient equal to $C1/PNB$ used during simultaneous solution of vessel equations
C1P	coefficient related to toluene diffusion which is used during simultaneous solution of vessel equations
C11	coefficient equal to acid phase mass transfer plus the sum of the reaction coefficients used during simultaneous solution of the vessel equations
C12	coefficient equal to $(- C1Ø - CR)$ used during simultaneous solution of the vessel equations
C21	coefficient equal to $(CA - C1A)$ used during simultaneous solution of the vessel equations
C22	coefficient equal to $(1 + C1Ø + CR)$ used during simultaneous solution of the vessel equations
C4	equal to the sum of reaction rates $R1$ thru $R6$. Represents the moles/hr water produced by reactions 1 thru 6
C5	moles/hr nitrosylsulfuric acid produced by oxidation reactions
C5P	net moles/hr nitrosylsulfuric acid produced after decomposition takes place

Q

C6	organic phase nitric acid solubility coefficient
DD (I)	rate of diffusion of organic component i. Used only in check calculations
DLA	convergence tolerance for components in both acid and organic phases flowing from the vessel currently being simulated
DRM	difference in molar densities between the acid and organic phases used in the entrainment correlation
D1	moles/hr of α MNT which diffuse from the organic into the acid phase in the vessel currently being simulated. Negative values means diffusion is from acid to organic phase
D10	moles/hr of toluene which diffuse from the bulk organic phase to the acid-organic interface
D2	same as D1 but for mMNT
D3	same as D1 but for α DNT
D4	same as D1 but for mDNT
D5	same as D1 but for α TNT
D6	same as D1 but for mTNT
D7	same as D1 but for TNBX
D8	same as D1 but for TNE
EAQ4	molar ratio of acid phase in the organic stream to total organic stream, based on the entrainment correlation
ETA	overall mass transfer coefficient in the vessel currently being simulated

ETAA	acid phase mass transfer coefficient in the vessel currently being simulated
ETAP	organic phase mass transfer coefficient in the vessel currently being simulated
ETATL	mass transfer coefficient for toluene in the organic phase
EXX	ratio acid phase to organic phase in the organic stream, based on the entrainment correlation
F	initial concentration of nitric acid prior to establishment of equilibrium conditions in the vessel currently being simulated
FA	volume fraction acid phase in the vessel currently being simulated
FACT	relaxation factor used in convergence procedure for composition of phases flowing from the vessel currently being simulated
FAR	fraction of the total acid phase flowing from a separator that is recycled for the separator currently being simulated
FAR1	fraction of the total acid phase flowing from a separator that is entrained in the organic stream which flows to the next nitrator for the separator currently being simulated
FC	constant equal to $(2 \times F) - C$ used in computation of nitronium ion equilibrium concentration in region 2 for the vessel currently being simulated
FF (I)	cross sectional area fraction corresponding to the i th notch setting on the gate valve in the internal recycle line of the separator currently being simulated

FHG	upper boundary value of internal recycle fraction computed using the entrainment coefficient
FIR	internal recycle fraction computed using the entrainment correlation for the separator currently being simulated
FLW	same as FHG except lower boundary value
FQG	molar ratio of organic phase in the acid recycle streams to total organic phase flowing from the separator currently being simulated (based on entrainment correlation)
FOGC	current value of FQG
FP	volume fraction of organic phase in the vessel currently being simulated
FPQ	molar fraction of the total organic phase flowing from a separator which appears in the organic stream for the separator currently being simulated
FPQ1	molar fraction of the total organic phase flowing from a separator which appears in the recycled acid streams for the separator currently being simulated
FR	volume fraction of the combined recycled acid streams which is external recycle for the separator currently being simulated
FRAC	volume fraction of the combined recycled acid streams which is internal recycle for the separator currently being simulated
FVKM	volume of the vessel currently being simulated
GAMMA	acid concentration factor for all nitration reactions in the vessel currently being simulated

G1	equivalent to F1(I) where I is the index of the nitrator currently being simulated or the index of the nitrator preceding the separator currently being simulated
G10	same as G1 but for F10(I)
G10P	rate of reaction 10 per mole of TNT in the acid phase flowing from the vessel currently being simulated
G15P	equivalent to G15(I) where I is the index of the vessel currently being simulated
G3	same as G1 but for F3(I)
G3D	rate of reaction 3 per mole of α MNT in the acid phase flowing from the vessel currently being simulated
G3S	same as G1 but for F3S(I)
G4	same as G1 but for F4(I)
G4D	rate of reaction 4 per mole of mMNT in the acid phase flowing from the vessel currently being simulated
G4S	same as G1 but for F4S(I)
G5	same as G1 but for F5(I)
G5G	rate of reaction 5 per mole of α DNT in the acid phase flowing from the vessel currently being simulated
G6	same as G1 but for F6(I)
G6G	rate of reaction 6 per mole of mDNT in the acid phase flowing from the vessel currently being simulated

G7	same as G1 but for F7 (I)
G7G	rate of reaction 7 per mole of DNT in the acid phase flowing from the vessel currently being simulated
G8	same as G1 but for F8 (I)
G8P	rate of reaction 8 per mole of DNT in the acid phase flowing from the vessel currently being simulated
G9	same as G1 but for F9 (I)
G9G	zero
ICOUNT	number of passes made through subroutine VESSEL during a particular convergence iteration for the vessel currently being simulated
ITR	number of convergence iterations executed for the vessel currently being simulated. Five iterations, each consisting of NC passes through VESSEL are allowed
MWAVGA	average molecular weight of the acid phase flowing from the separator which is being simulated and for which entrainment is being determined via the correlation
MWAVGP	same as MWAVGA but for the organic phase
NC	maximum number of passes through VESSEL allowed per iteration during vessel equation convergence procedure
NQTCH	value of $NQ(I)$ where I is the index of the separator currently being simulated
P (I)	moles/hr of component i in the organic phase flowing from the vessel currently being simulated

PNB	moles/hr of combined organic components in the organic phase flowing from the vessel currently being simulated
PP	exponent of the nitrobody-in-acid solubility correlation
PT	moles/hr of combined organic components in both the acid and organic phases flowing from the vessel currently being simulated
PTI	the reciprocal of PT. Used for computation of entrainment via the correlation
PX(I)	same as P(I) for components 1 thru 8 but used only in check calculations
PX10	same as P(10) but used only in check calculations
PX9	same as P(9) but used only in check calculations
P1	moles/hr α MNT in the organic phase flowing from the vessel currently being simulated
P10	same as P1 but for toluene
P2	same as P1 but for mMNT
P3	same as P1 but for α DNT
P4	same as P1 but for mDNT
P5	same as P1 but for α TNT
P6	same as P1 but for mTNT
P7	same as P1 but for TNBX
P8	same as P1 but for TNB
P9	same as P1 but for nitric acid

Q	fraction of molecular nitric acid converted to nitronium ion in the vessel currently being simulated
QA	ft ³ /hr of acid phase flowing from the vessel currently being simulated
QP	ft ³ /hr of organic phase flowing from the vessel currently being simulated
QT	volumetric flow (ft ³ /hr) of combined internal plus external recycle streams flowing from the separator currently being simulated
RHLO	mass density (lb/ft ³) of the organic phase flowing from the separator currently being simulated and for which entrainment is being determined via the correlation
RHQO	same as RHLO but molar density (moles/ft ³)
RR1	same as R1 but used only for check calculation
RR10	same as R10 but used only for check calculation
RR3	same as RR1 but for R3
RR7	same as RR1 but for R7
RR8	same as RR1 but for R8
RR9	same as RR1 but for R9
RR9G	same as RR1 but for R9G
RTL	mass ratio of organic to acid phase in the separator currently being simulated and for which entrainment is being calculated via the correlation
RTO	same as RTL but molar ratio

RVOL	maximum volumetric flow of internal recycle stream possible for a given notch setting in the separator currently being simulated and for which entrainment is being calculated via the correlation
R10A	rate of reaction 10 for α TNT in the vessel currently being simulated
R10M	rate of reaction 10 for mTNT in the vessel currently being simulated
R7A	rate of reaction 7 for mDNT in the vessel currently being simulated
R8A	rate of reaction 8 for α DNT in the vessel currently being simulated
R8M	rate of reaction 8 for mDNT in the vessel currently being simulated
R9G	zero
R9GA	zero
R9GM	zero
S	initial concentration (moles/ft ³) of total sulfuric acid in the acid phase of the vessel currently being simulated
SANB	same as ANB but used only in check calculations
SANBC	same as SANB but based on computed solubility
SPNB	same as PNB but used only in check calculations
SUM	sum of the individual organic component diffusions used only in the check calculations
TAF	moles/hr of entrained acid phase (based on the correlation) contained in the organic stream flowing from the separator currently being simulated

TAIR	moles/hr of acid phase (based on the correlation) contained in the internal recycle stream flowing from the separator currently being simulated
TAR	moles/hr of acid phase (based on the correlation) contained in the combined internal and external recycle streams flowing from the separator currently being simulated
TAXR	moles/hr of acid phase (based on the correlation) contained in the external recycle stream flowing from the separator currently being simulated
TKEL	temperature (in Degrees Kelvin) of the vessel currently being simulated
TLI	total mass flow (lb/hr) through the separator currently being simulated and for which entrainment is being computed via the correlation
TPF	moles/hr of organic phase (based on the correlation) contained in the organic stream flowing from the separator currently being simulated
TPIR	moles/hr of entrained organic phase (based on the correlation) contained in the internal recycle stream flowing from the separator currently being simulated
TPR	moles/hr of entrained organic phase (based on the correlation) contained in the combined recycle streams flowing from the separator currently being simulated
TPXR	moles/hr of entrained organic phase (based on the correlation) contained in the external recycle stream flowing from the separator currently being simulated

V0(I)	storage vector for the values of the i component molar flows generator on the previous pass through VESSEL for the vessel currently being simulated
W	concentration (moles/ft ³) of water in the vessel currently being simulated
X	computed equilibrium concentration of nitronium ion in the acid phase under aqueous conditions and under conditions of oleum region 3. Also equilibrium concentration at molecular nitric acid in oleum region 2
XA	NOT USED
XB	NOT USED
XC	NOT USED
AD	NOT USED
XE	NOT USED
XEQA	equilibrium solubility of organic material (nitrobody) in the acid phase of the vessel currently being simulated
XF	NOT USED
XL	lower boundary value used in an interval halving convergence procedure
XU	upper boundary valued used in an interval halving convergence procedure
X1	mole fraction α MNT in the acid phase of the vessel currently being simulated
X11	same as X1 but for sulfuric acid
X12	same as X1 but for nitrosylsulfuric acid

U

X13	same as X1 but for water
X14	same as X1 but for SO ₂
X2	same as X1 but for mMNT
X3	same as X1 but for α DNT
X4	same as X1 but for mDNT
X5	same as X1 but for α TNT
X6	same as X1 but for mTNT
X7	same as X1 but for TNBX
X8	same as X1 but for TNB
X9	same as X1 but for nitric acid
Y	equilibrium concentration of the pyrosulfate ion in the acid phase of the vessel being simulated under conditons of oleum region 3
YL	lower boundary value used in an interval halving convergence procedure
YU	upper boundary value used in an interval halving convergence procedure
Y1	mole fraction of α MNT in the organic phase of the vessel currently being simulated
Y10	same as Y1 but for toluene
Y2	same as Y1 but for mMNT
Y3	same as Y1 but for α DNT
Y4	same as Y1 but for mDNT
Y5	same as Y1 but for α TNT

Y6	same as Y1 but for MTNT
Y7	same as Y1 but for TNBX
Y8	same as Y1 but for TNB
Y9	same as Y1 but for nitric acid
ZA	diffusion coefficient for organic components in the organic phase
ZB	diffusion coefficient for organic components in the acid phase

Function ENTH

The definitions of the following variables are identical to those in the main program: AKA, AKEQ, AKMA, AKMATL, AK10, AK12, AK3S, AK3W, AK4S, AK4W, AK5S, AK6S, AK7, AK8, CP(I), DH(I), E10, E21, E3S, E3W, E4S, E4W, E5S, E6S, E7, E8, FD, FMAX, RH01, RH010, RH011, RH012, RH013, RH014, RH02, RH03, RH04, RH05, RH06, RH07, RH08, RH09, RP, RR, SA, SB, SC, SD, SE, SG, SH, SI, SJ, TR

Remaining variables are defined as follows:

A(I)	moles/hr of component i in the acid phase of the stream for which the enthalpy is currently being calculated
CP11	equivalent to CP(11)
CP12	equivalent to CP(12)
CP13	equivalent to CP(13)
CP14	equivalent to CP(14)
CP9	equivalent to CP(9)
DLT	temperature of the vessel (relative to 20°C) for which the enthalpy of a particular exiting stream is currently being calculated

ENTH	enthalpy of the stream currently being calculated (kcal/hr)
ENTHQ	enthalpy of mixing of the acid components in the acid phase of the stream currently being calculated based on the zero nitric curve of the McKinley and Brown data (kcal/lb)
ENTH2	same as ENTHQ but based on the 20% nitric curve
F	adjusted weight fraction (nitrobody free basis) of nitric plus equivalent sulfuric acid in the acid phase of the stream currently being calculated
I	general index integer
J	general index integer
LBS	lb/hr of nitric acid, sulfuric acid, water and SO ₂ flowing with the acid phase of the stream for which the enthalpy is currently being calculated
LBSE	lb/hr of nitric acid plus equivalent sulfuric acid in the acid phase of the stream for which the enthalpy is currently being calculated
P(I)	moles/hr of component i in the organic phase of the stream for which the enthalpy is currently being calculated
T	moles/hr of a given organic component in the combined acid and organic phases (i.e., in the total stream) of the stream for which the enthalpy is currently being calculated
TP	temperature of the vessel for which the enthalpy of a particular exiting stream is being calculated
WTA	LBSE/LBS; nitrobody free weight fraction of nitric plus equivalent sulfuric acid in the acid phase of the stream for which the enthalpy is currently being calculated

WTN	weight fraction of nitric acid in the nitric plus equivalent sulfuric acid portion of the acid phase of the stream for which the enthalpy is currently being calculated
X(I)	the <i>i</i> th data point on the zero % nitric curve from the enthalpy-concentration data of McKinley and Brown
Y(I)	the <i>i</i> th data point on the 20% nitric curve from the enthalpy-concentration data of McKinley and Brown

APPENDIX I

Steady State Simulation--Input Data Format

CARD	DATA READ	FORMAT
1	AK12, AK3W, AK4W, AK5S, AK6S, AK7, AK8, AK10	8F10.0
2	AK3S, AK4S, E3S, E4S	8F10.0
3	E21, E3W, E4W, E5S, E6S, E7, E8, E10	8F10.0
4	SA, SB, SC, SE, SG, SH, SI	8F10.0
5	SJ, RR, TR, AKMA, AKMATL, FMAX FD, RP	8F10.0
6	AKA, AKS, AKC, AKEQ, AKEQOV, FOV	8F10.0
7, 8	AVI(I,1), I=1,14	8F10.0/8F10.0
9,10	PVI(I,1), I=1,14	8F10.0/8F10.0
11,12	AVI(I,2), I=1,14	8F10.0/8F10.0
13,14	PVI(I,2), I=1,14	8F10.0/8F10.0
15,16	AVI(I,3), I=1,14	8F10.0/8F10.0
17,18	PVI(I,3), I=1,14	8F10.0/8F10.0
19,20	AVI(I,4), I=1,14	8F10.0/8F10.0
21,22	PVI(I,4), I=1,14	8F10.0/8F10.0
23,24	AVI(I,5), I=1,14	8F10.0/8F10.0
25,26	PVI(I,5), I=1,14	8F10.0/8F10.0
27,28	AVI(I,6), I=1,14	8F10.0/8F10.0
29,30	PVI(I,6), I=1,14	8F10.0/8F10.0
31,32	AVI(I,7), I=1,14	8F10.0/8F10.0
33,34	PVI(I,7), I=1,14	8F10.0/8F10.0
35,36	AVI(I,8), I=1,14	8F10.0/8F10.0
37,38	PVI(I,8), I=1,14	8F10.0/8F10.0
39,40	AVI(I,9), I=1,14	8F10.0/8F10.0
41,42	PVI(I,9), I=1,14	8F10.0/8F10.0
43,44	AVI(I,10), I=1,14	8F10.0/8F10.0

CARD	DATA READ	FORMAT
45,46	PVI(I,10), I=1,14	8F10.0/8F10.0
47,48	AVI(I,11), I=1,14	8F10.0/8F10.0
49,50	PVI(I,11), I=1,14	8F10.0/8F10.0
51,52	AVI(I,12), I=1,14	8F10.0/8F10.0
53,54	PVI(I,12), I=1,14	8F10.0/8F10.0
55,56	AVI(I,13), I=1,14	8F10.0/8F10.0
57,58	PVI(I,13), I=1,14	8F10.0/8F10.0
59,60	AVI(I,14), I=1,14	8F10.0/8F10.0
61,62	PVI(I,14), I=1,14	8F10.0/8F10.0
63	FACT 6, FACT 5, FACT 4, FACT 3, FACT 2	5F10.0
64	NDA	I2
65	TITLE	20A4
66	IPRNT, EI, ILIST, IMBAL, IPI, IAFI, IPNCH, ICHECK	9I1
67	FIN(1,J), J=1,8	8F10.0
68	FIN(2,J), J=1,8	8F10.0
69	FIN(3,J), J=1,8	8F10.0
70	FIN(4,J), J=1,8	8F10.0
71	FIN(5,J), J=1,8	8F10.0
72	FIN(6,J), J=1,8	8F10.0
73	FIN(7,J), J=1,8	8F10.0
74-83	((COMP(J,I), I=1,14), J=1,5)	8F10.0/8F10.0
84	NO(I), I=1,8	6I
85	TEMP(I), I=1,8	8F10.0
86	VKM(I), I=1,8	8F10.0
87	VKMS	F10.0
88	EQO(I), I=1,8	8F10.0
89	EQA(I), I=1,8	8F10.0

APPENDIX J
Parameter Fitting

Table J1

Nitration snapshot

B-Line - 8/18/71 - 1:30 pm

	<u>Nitrator Temperature</u>	<u>Separator Temperature</u>	<u>Recycle Setting</u>	<u>Weak Nitric Flows, lbs/hr</u>	<u>Strong Nitric Flows, lbs/hr</u>
1A	51	51		500 from Fume Recovery 2445 from SAR	
1B	44	51	1		
2	76	66	1	3467 from SAR	7
3A	80				43
3B	86	78	5		202
4	89	94	2		144
5	96	103	2		1118
6	104	104	1		
Toluene	2418 lbs/hr				
Oleum	12300 lbs/hr				
			No fresh water added		
			Yellow water to 1A - 1200 lbs/hr		

Acid Analysis - Acid Phase

	<u>Yellow Water</u>	<u>Spent</u>	<u>1B</u>	<u>2</u>	<u>3B</u>	<u>4</u>	<u>5</u>	<u>6</u>
Total Acidity	11.97	74.68	72.78	88.49	98.26	100.86	103.28	103.17
Total Sulfuric	8.28	67.22	66.67	78.65	84.93	88.32	90.53	90.95
Actual Nitric	4.76	3.63	5.89	10.60	13.86	13.97	15.15	15.42
HNOSO ₄		12.00	1.96	4.11	6.58	4.33	2.50	0.57
Water	86.98	23.41	26.54	9.81	-0.29	-3.28	-6.16	-6.50
Nitrobody		0.38	0.49	7.12	23.18	16.12	19.04	20.27
Acid Density			1.619	1.716		1.786	1.798	1.790

Table J1 (Cont'd)

Acid Analysis - Nitrobody Phase

	<u>1B</u>	<u>2</u>	<u>3B</u>	<u>4</u>	<u>5</u>	<u>6</u>
Total Acidity	4.88	9.37	4.88	1.06	0.71	0.16
Total Sulfuric	0.70	1.51	1.54	0.61	0.60	0.12
Actual Nitric	4.97	9.98	3.96	0.28	0.14	0.05
HNOSO ₄	0.81	0.24	0.66	0.66	0.33	0
Water and Nitrobody	99.42	88.33	93.99	98.99	99.17	99.83
Separator Density	1.208	1.366	1.430			

Gas Analysis

	<u>Gas Chromatography - Percentage by Volume</u>					<u>Total Toluene Loss</u>
	<u>CO₂</u>	<u>O₂</u>	<u>N₂</u>	<u>CO</u>	<u>N₂O</u>	
Sample 1	6.89	17.62	63.38	5.07	0.46	7.5
Sample 2	6.24	17.84	63.31	4.21	0.37	6.5
Total Gas Flow - 687 cu ft/min						

MSA
Billionaire
NO_x

TNM
610
490

Acid PhaseOxidation Products (Wt %)

<u>Compound</u>	<u>Spent Acid</u>				
	<u>1B</u>	<u>2</u>	<u>3B</u>	<u>4</u>	<u>5</u>
Trinitrobenzene	0.50	0.04	0.22	0.14	0.01

Table J1 (Cont'd)

Compound	Spent Acid	Nitrobody in Acid Phase					
		1B	2	3B	4	5	6
2-MNT	25.67	43.93					
3-MNT	1.94	3.04					
4-MNT	19.04	28.36					
TOTAL MNT	46.65	75.33					
*PNM	2.06						
2,6-DNT	5.72	3.67	10.63	3.28	0.54	0.06	0.01
2,5-DNT	0.19	0.07	6.56	0.31	0.12	0.03	0.05
2,4-DNT	33.03	16.75	84.50	36.42	10.99	1.50	0.16
3,5-DNT			0.84	0.03	0.01		0.04
3,4-DNT			96.53	0.37	0.05	0.01	
TOTAL DNT	38.94	20.49		40.41	11.71	1.60	0.26
2,4,6-TNT	11.84	4.13	2.85	57.89	86.20	95.72	96.69
2,3,5-TNT				0.02	0.02	0.04	0.05
2,4,5-TNT			0.33	1.16	1.49	1.76	2.02
2,3,4-TNT			0.96	0.39	0.57	0.84	1.01
TOTAL TNT	11.84	4.13	3.24	59.46	88.28	98.36	99.72

*PNM - phenylnitromethane resulting from methyl group nitration of toluene

Table J1 (Cont'd)

Compound	Nitrobody Phase					
	Oxidation Products (Wt %)					
	1B	2	3B	4	5	6
Trinitrobenzene	0.02	0.30	0.37	0.25	0.19	0.08
Analysis of Nitrobody Phase						
Compound	1B	2	3B	4	5	6
Toluene	0.28					
2-MNT	45.98					
3-MNT	2.87					
4-MNT	28.26					
TOTAL MNT	77.11					
2,6-DNT	2.31	10.99	4.13	0.89	0.10	0.01
2,5-DNT	0.12	0.47	0.13	0.13	0.04	0.01
2,4-DNT	15.65	58.12	25.35	9.12	1.47	0.16
3,5-DNT			0.02	0.01	0.001	0.04
3,4-DNT	0.12	1.28	0.55	0.12	0.01	
TOTAL DNT	18.20	70.86	30.36	10.27	1.62	0.22
2,4,6-TNT	4.23	28.50	66.92	86.39	94.64	98.00
2,3,5-TNT			0.02	0.03	0.05	0.06
2,4,5-TNT		0.25	1.64	2.05	2.29	2.32
2,3,4-TNT		0.10	0.69	1.02	1.22	1.33
TOTAL TNT	4.23	28.85	69.27	89.49	98.20	99.71
Separator - Density	1.208	1.366	1.430			

Table J2

Final values of parameters

Parameter	Coded Name	Value	Units
k_{12}	AK12	88.9	dimensionless
k_{3s}	AK3S	1.8×10^7	hr^{-1}
k_{4s}	AK4S	1.0×10^7	hr^{-1}
k_{55s}	AK5S	124.5	hr^{-1}
k_{6s}	AK6S	506.8	hr^{-1}
k_7	AK7	.09	hr^{-1}
k_8	AK8	2.1	hr^{-1}
k_{10}	AK10	.001	hr^{-1}
k_a	AKA	.2	$(\text{ft}^3) (\text{lb-moles})^{-1}$
K_{eq1}	SH	.03	$(\text{lb-moles}) (\text{ft}^3)^{-1}$
K_{eq2}	AKEQ	50.	dimensionless
K_{eq3}	SJ	6.0×10^4	$(\text{lb-moles})^2 (\text{ft}^3)^{-2}$
K_{eq4}	SC	0.	$(\text{ft}^3) (\text{lb-moles})^{-1}$
E_{21}	E21	88.9	$(\text{Kcal}) (\text{lb-mole})^{-1}$
E_{3s}	E3S	2.2×10^4	$(\text{Kcal}) (\text{lb-mole})^{-1}$
E_{4s}	E4S	1.0×10^4	$(\text{Kcal}) (\text{lb-mole})^{-1}$
E_{5s}	E5S	9.3×10^3	$(\text{Kcal}) (\text{lb-mole})^{-1}$
E_{6s}	E6S	6.5×10^3	$(\text{Kcal}) (\text{lb-mole})^{-1}$
E_7	E7	5.0×10^3	$(\text{Kcal}) (\text{lb-mole})^{-1}$

Parameter	Coded Name	Value	Units
E_8	E8	7.0×10^3	(Kcal) (lb-mole) ⁻¹
E_{10}	E10	1.0	(Kcal) (lb-mole) ⁻¹
k_m^a	AKMA	2.75×10^4	$[(\text{lb-moles}) (\text{hr})^{-1} (\text{ft}^2)^{-1}] \times$ $[(\text{ft}^3) (\text{ft}^3)^{-1}]$
$(k_m^a)_p$	AKMAP	1.55×10^4	$[(\text{lb-moles}) (\text{hr})^{-1} (\text{ft}^2)^{-1}] \times$ $[(\text{ft}^3) (\text{ft}^3)^{-1}]$
$(k_m^a)_{\text{Tol}}$	AKMATL	5.0×10^3	$[(\text{lb-mole}) (\text{hr})^{-1} (\text{ft}^2)^{-1}] \times$ $[(\text{ft}^3) (\text{ft}^3)^{-1}]$
i	SI	1.51	dimensionless
F_D	FD	.65	dimensionless
RP	RP	.6	dimensionless

APPENDIX K

Steady State Optimization

Table K1
Independent variables

Variable	Rank
Weak Nitric Acid to 1A	6
Weak Nitric Acid to 1B	20
Weak Nitric Acid to 2	5
Fume Recovery Nitric Acid to 1A	18
Fume Recovery Nitric Acid to 1B	19
Yellow Water to 1A	22
Yellow Water to 1B	28
Yellow Water to 2	17
Fresh Water to 1A	26
Fresh Water to 2	27
Strong Nitric Acid to 3A	4
Strong Nitric Acid to 3B	12
Strong Nitric Acid to 4	3
Strong Nitric Acid to 5	11
Strong Nitric Acid to 6	2
Oleum to 6	1
Concentration of Weak Nitric Acid	13
Concentration of Fume Recovery Nitric Acid	10
Concentration of Strong Nitric Acid	9
Sulfuric Content of Oleum	8
Temperature of Nitrator 1A	7
Temperature of Nitrator 1B	25
Temperature of Nitrator 2	21
Temperature of Nitrator 3A	14
Temperature of Nitrator 3B	15

Table K1 (Cont'd)

Variable	Rank
Temperature of Nitrator 4	23
Temperature of Nitrator 5	24
Temperature of Nitrator 6	16
Recycle Valve Notch Setting in Separator 1	32
Recycle Valve Notch Setting in Separator 2	31
Recycle Valve Notch Setting in Separator 3	29
Recycle Valve Notch Setting in Separator 4	30
Recycle Valve Notch Setting in Separator 5	33
Recycle Valve Notch Setting in Separator 6	34

Table K2

Constraint list

1. % DNT in Crude TNT must be less than .4
2. % Dissolved Nitrobody in Spent Acid $\leq .5$
3. % DNT in Dissolved Nitrobody ≤ 55 .
4. Weak Nitric Concentration $\leq 61\%$
5. Fume Recovery Concentration $\leq 58\%$
6. Strong Nitric Concentration $\leq 99\%$
7. % H_2SO_4 in Oleum $\geq 57\%$
8. Wt % Actual Nitric (AN) in stages 3-6 ≤ 16
9. AN(3) ≥ 7
10. AN(4) ≥ 8
11. AN(5,6) ≥ 10
12. AN(1) ≤ 6
13. AN(2) ≤ 11
14. AN(1) ≥ 2.5
15. AN(2) ≥ 4.5
16. $20. \leq$ [Temperature of Nitrator 1A (T1A)]
17. $20. \leq T1B \leq 60. ^\circ C$
18. $50. \leq T2 \leq 70. ^\circ C$
19. $60. \leq T3A \leq 100. ^\circ C$
20. $60. \leq T3B \leq 100. ^\circ C$
21. $70. \leq T4 \leq 110. ^\circ C$
22. $80. \leq T5 \leq 115. ^\circ C$
23. $90. \leq T6 \leq 120. ^\circ C$
24. Heat Load in Nitrator 1A $\leq 2.5 \times 10^6$ BTU/hr
25. $66. \leq$ (% Total Acidity of Spent Acid) $\leq 72.$

Table K3

Optimum operating conditions

Basis: 59.2 tons/day production rate
10000 lb/hr oleum feed rate

Nitrator	1A	1B	2	3A	3B	4	5	6
Weak Nitric	2000		1900					
Fume Recovery Nitric	600							
Yellow Water	1000							
Strong Nitric				600	500	400	100	1100
Oleum								10000
Toluene	1763	587						
Temperature	51	33	84	83	85	90	95	110

<u>Stage</u>	<u>Actual Nitric</u>	<u>Total Acidity</u>
1	3.1	70.9
2	6.1	85.0
3	11.1	93.6
4	13.5	101.2
5	13.6	103.6
6	13.9	104.2

Yield = 89.2%
DNT in crude TNT = .17%
Wt % dissolved nitrobody in spent acid = .3
Wt % of dissolved nitrobody which is DNT = 19.7
Raw Material Cost = 5.45¢/lb TNT

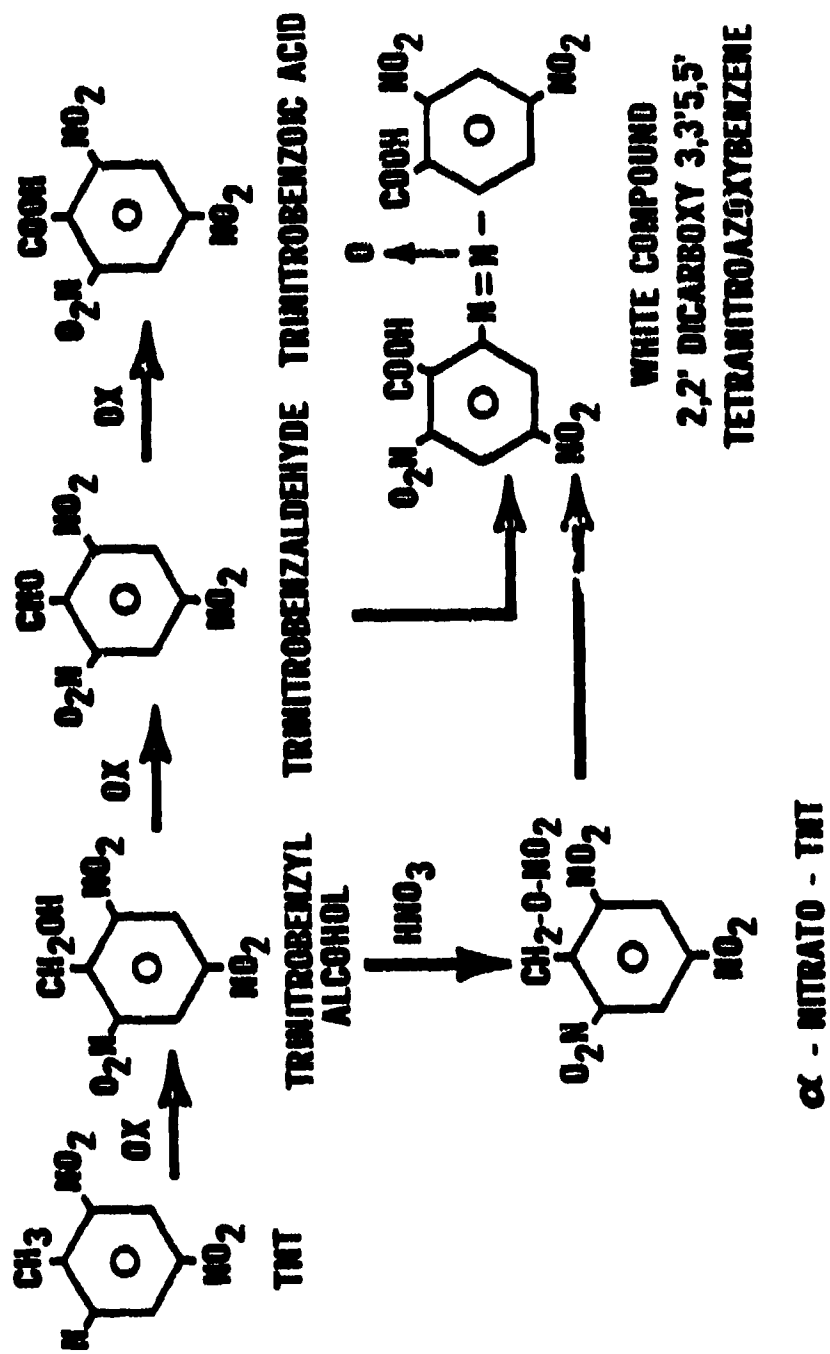


Fig 2 Oxidation of trinitrotoluene

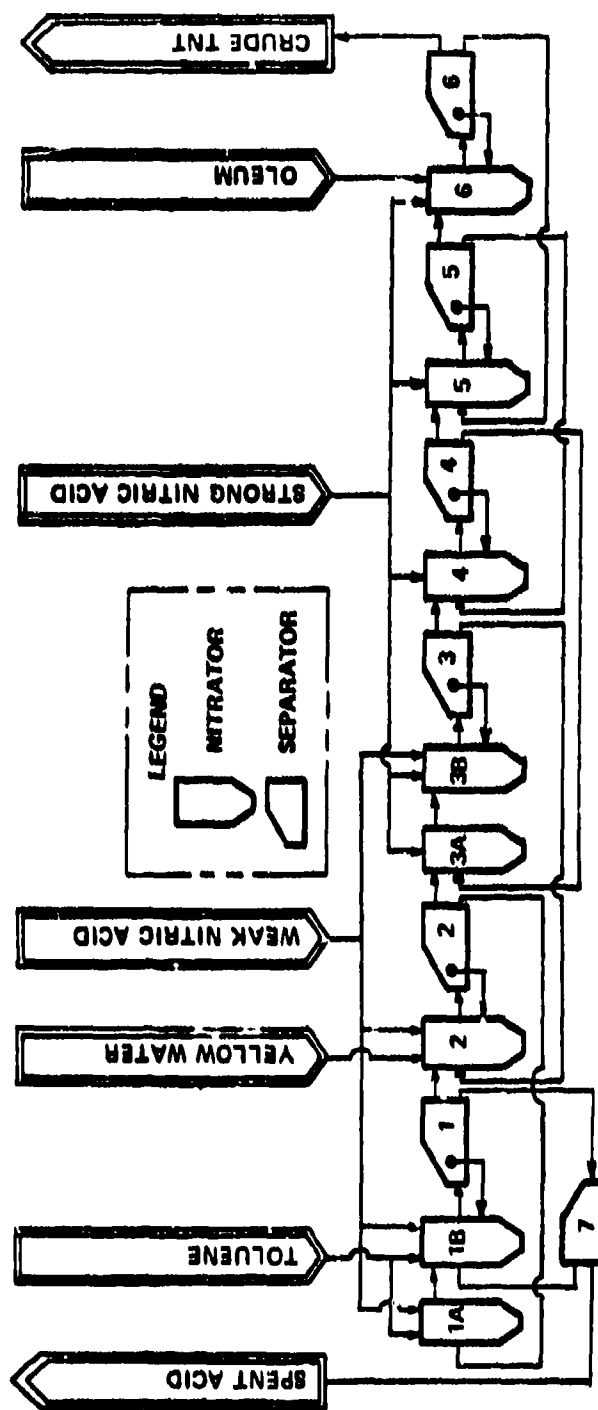


Fig 3 TNT nitration flow scheme (inter-vessel relationship)

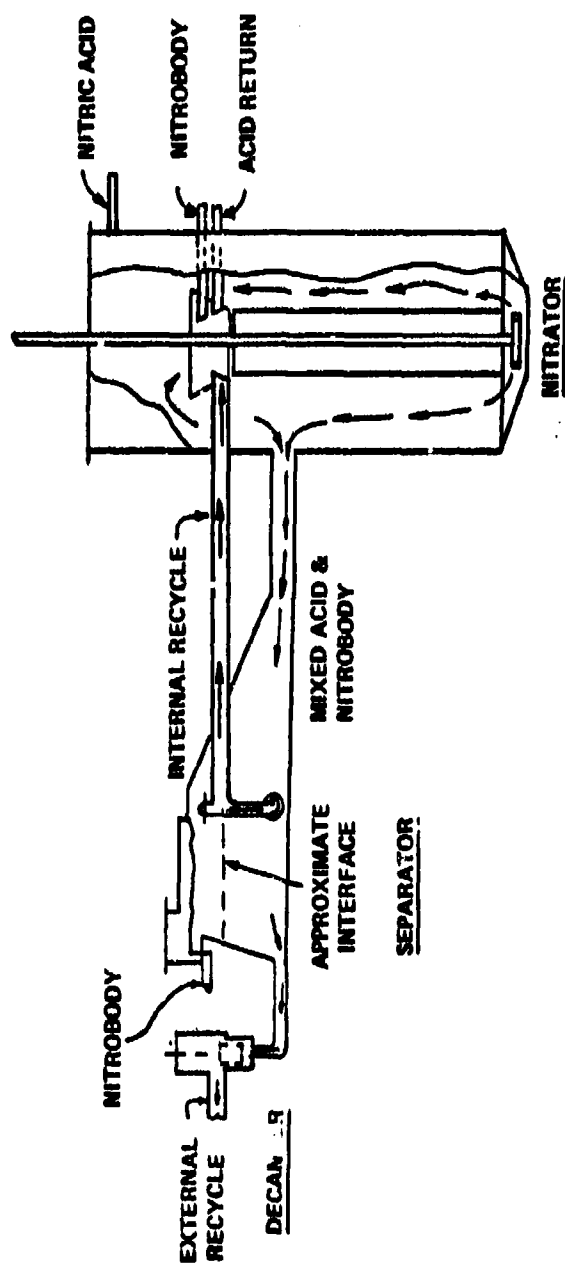
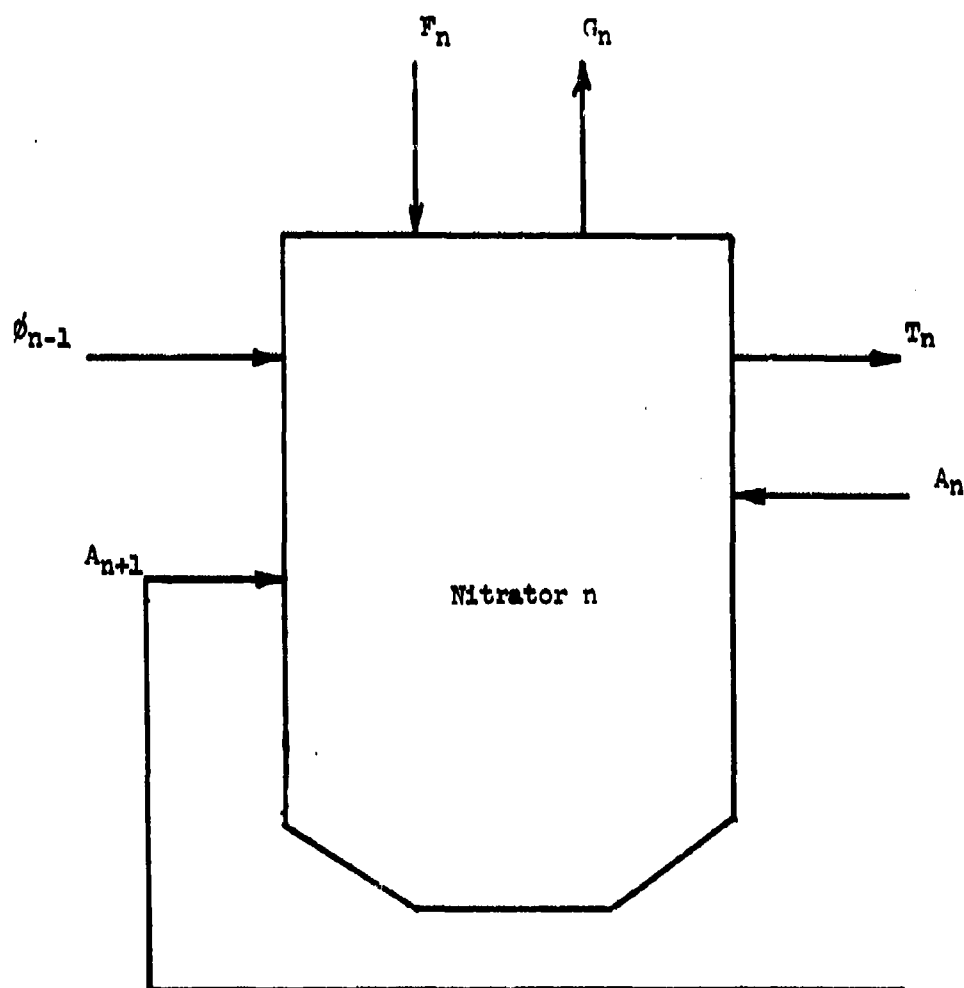


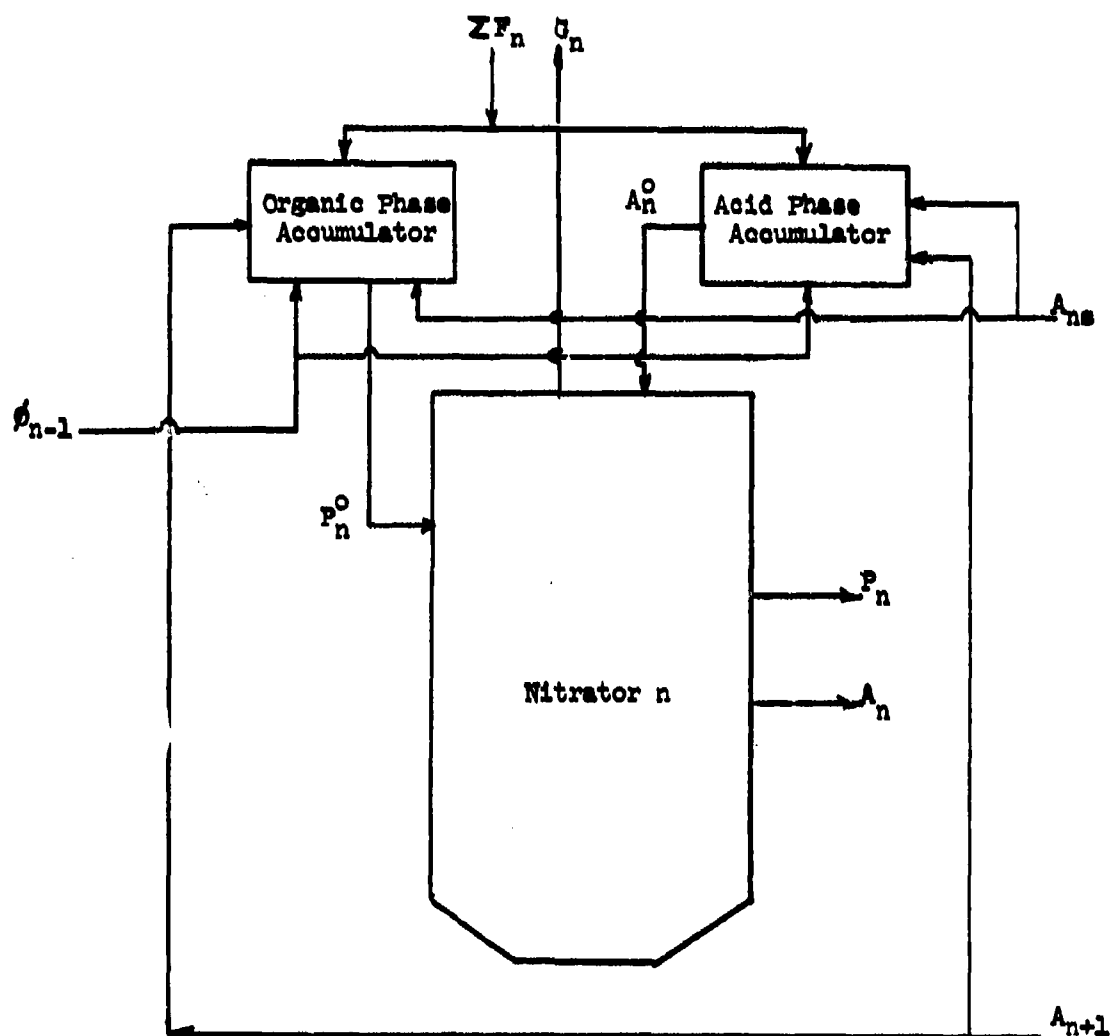
Fig 4 Nitration-separator combination



where:

- $\sum F_n$ = sum of fresh feeds to nitrator n
- ϕ_{n-1} = organic stream forward from separator n-1
- G_n = total off-gas
- A_{n+1} = acid recycle stream from separator n+1
- A_n = acid recycle stream from separator n
- T_n = total outflow from nitrator n

Fig 5 Generalized nitrator



where:

P_n^O = total organic phase input to nitrator n

A_n^O = total acid phase input to nitrator n

P_n = total organic phase output from nitrator n

A_n = total acid phase output from nitrator n

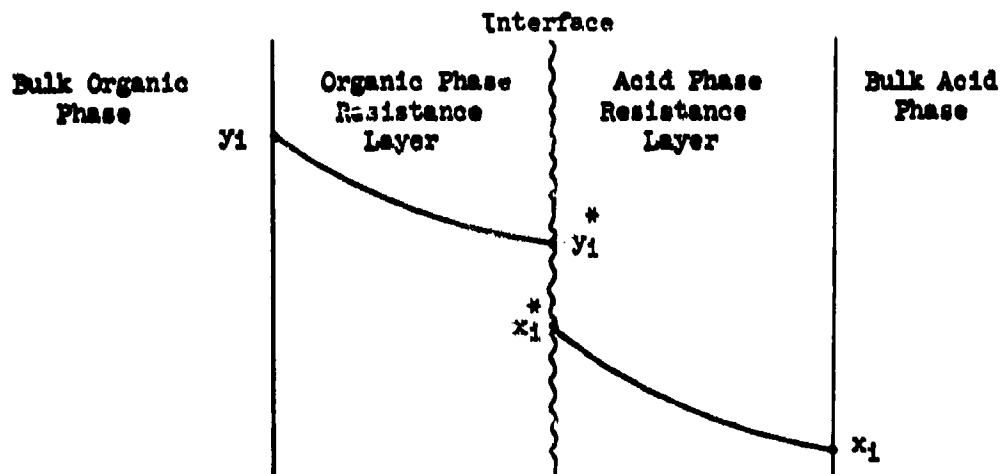
A_{ns} is equivalent to A_n in figure 5 and A_{n+1} . ϕ_{n-1} , G_n and ΣF_n are defined exactly as in figure 5

Fig 6 Simplified nitrator

CHEMICAL SPECIES CONSIDERED

ORGANIC PHASE	ACID PHASE	GAS PHASE
TOLUENE	TOLUENE	NO _x
o - MNT	o - MNT	CO _x
m - MNT	m - MNT	TNM
o - DNT	o - DNT	
m - DNT	m - DNT	
o - TNT	o - TNT	
m - TNT	m - TNT	
TNB	TNB	
TNBX	TNBX	
HNO ₃	HNO ₃	
	H ₂ SO ₄	
	H ₂ O	
	SO ₃	
	HNO ₃ SO ₄	

Fig 7 Chemical components considered in the model



- D_1 - net rate of diffusion of species 1 into the acid phase
- y_1 - mole fraction species 1 in bulk organic phase
- x_1 - mole fraction species 1 in bulk acid phase
- x_{eq}^A - equilibrium solubility of all organic species in the acid phase
or mole fraction organic species in acid phase at saturation
- η_ϕ - mass transfer coefficient in acid phase
- η_A - mass transfer coefficient in organic phase
- A_1 - moles species 1 in acid phase
- ϕ_1 - moles species 1 in organic phase
- A_T - total moles in acid phase
- ϕ_T - total moles in organic phase
- A_{NB} - total moles of nitrobody in acid phase
- ϕ_{NB} - total moles of nitrobody in organic phase
- $*$ - superscript denoting equilibrium at the interface

Fig 8 Diffusion in the nitration process

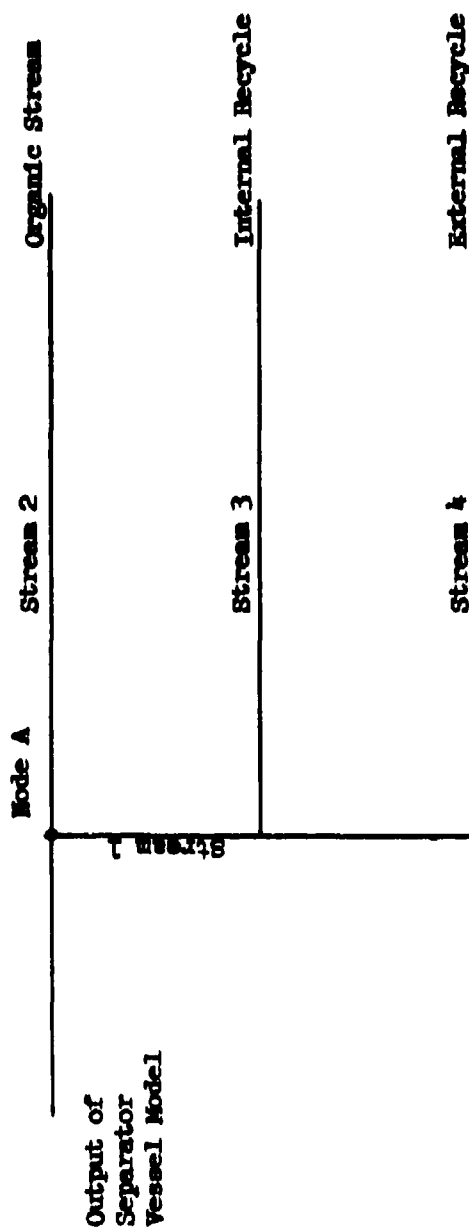


Fig 9 The separation process

LIST OF VARIABLES

Manipulated Variable	Controlled Variable
1. Water to Stage 1	Total Acidity, Stage 1
2. Weak Nitric to Stage 1	Nitric Concentration, Stage 1
3. Water to Stage 2	Total Acidity, Stage 2
4. Weak Nitric to Stage 2	Nitric Concentration, Stage 2
5. Strong Nitric to Stage 3A	Nitric to Sulfuric Ratio, Nitrator 3A
6. Strong Nitric to Stage 3B	Nitric to Sulfuric Ratio, Stage 3B
7. Strong Nitric to Stage 4	Nitric to Sulfuric Ratio, Stage 4
8. Strong Nitric to Stage 5	Nitric to Sulfuric Ratio, Stage 5
9. Strong Nitric to Stage 6	Nitric to Sulfuric Ratio, Stage 6

Fig 10 Acid concentration control--variables operated on

Block Diagram

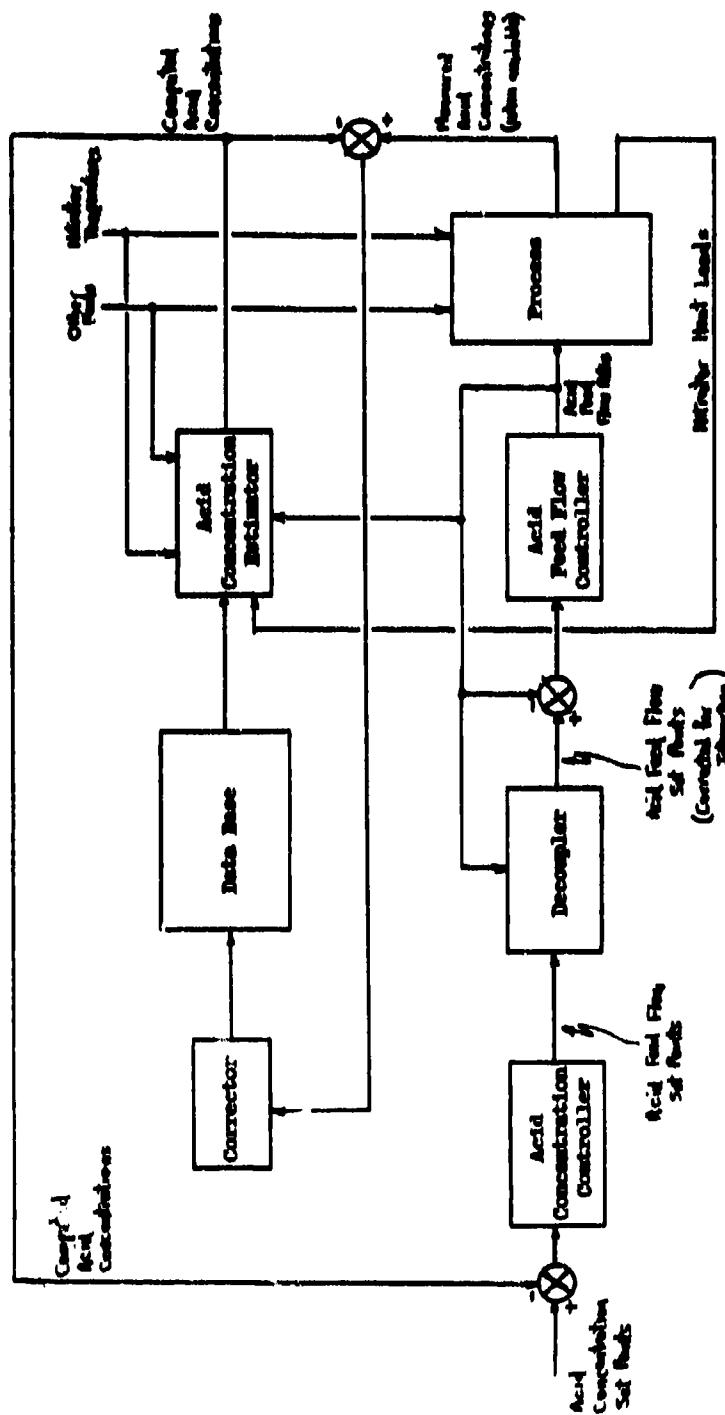


Fig 11 Acid concentration control--schematic diagram

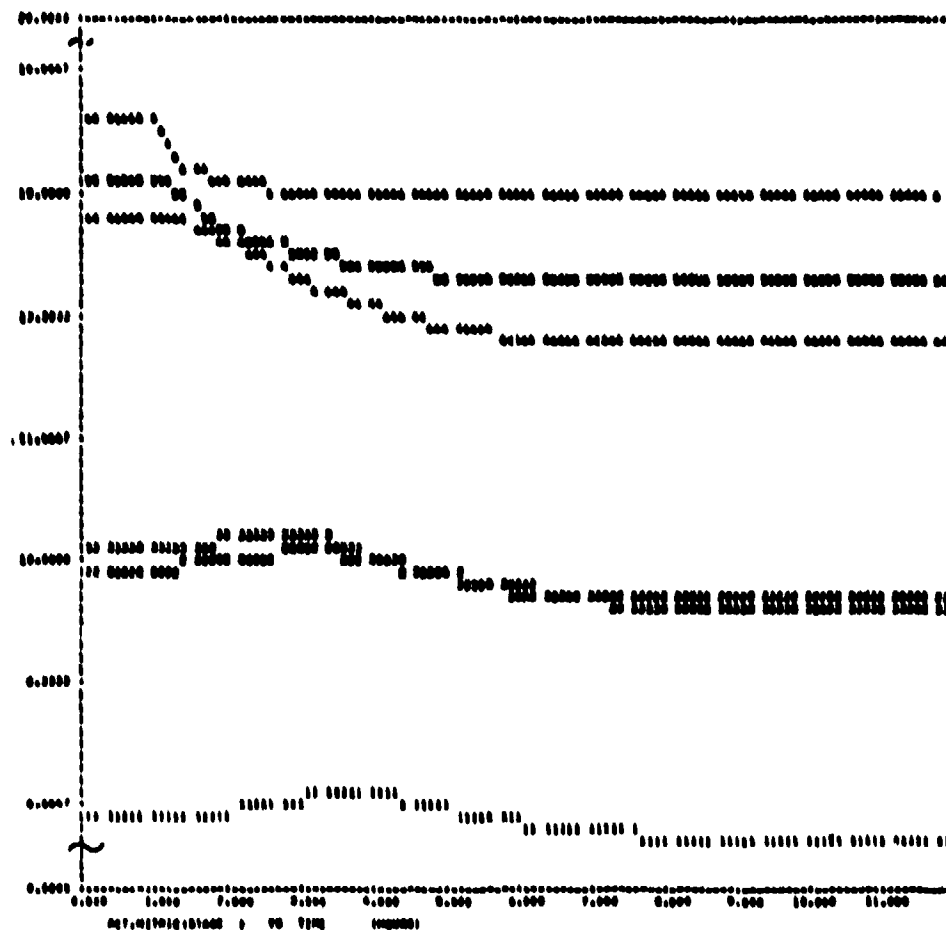


Fig 12 Open loop response of dynamic simulation

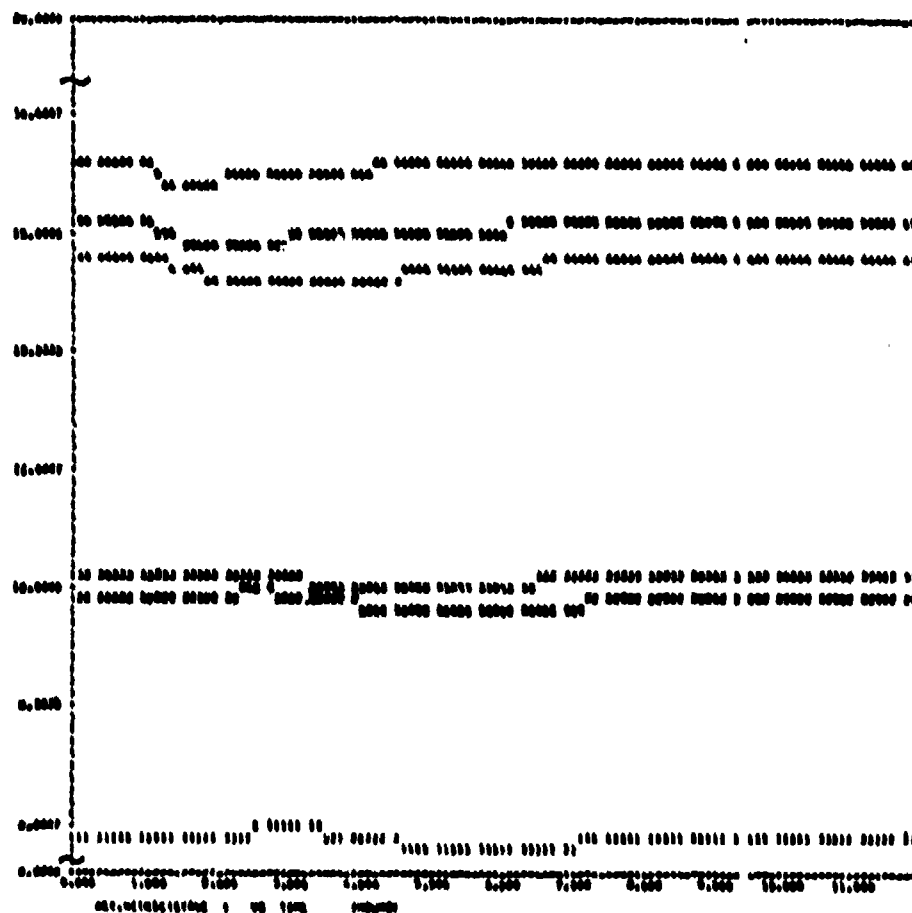


Fig 13 Response of dynamic simulation under acid concentration control